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SEARCH REQUEST FORM

Requester's Full Name: MARK BACH Examiner #: 59193 Date: 3/6/07  
Art Unit: 1624 Phone Number: 2-0663 Serial Number: 10511537  
Location (Bldg/Room#): 5C01 (Mailbox #): 5C18 Results Format Preferred (circle): PAPER DISK  
\*\*\*\*\*

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: \_\_\_\_\_

Inventors (please provide full names): \_\_\_\_\_

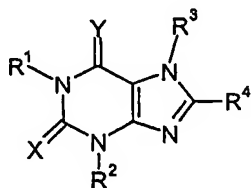
03-298

Earliest Priority Date: \_\_\_\_\_

Search Topic:

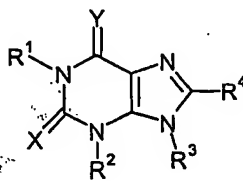
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.



(Ia)

or



(Ib)

wherein:

one of X and Y represents S, and the other represents O or S;

R<sup>1</sup> represents hydrogen or C1 to 6 alkyl;

R<sub>3</sub>, R<sub>4</sub>  
R<sub>2</sub> = H | C<sup>L1</sup>=C<sup>L2</sup>-C<sup>L3</sup>  
↑ chain must have only single bonds attached  
L<sub>1</sub>, L<sub>2</sub>, L<sub>3</sub> = H | C | O

20070312-10511537-str. rtf

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Searcher: MB

Searcher Phone #: \_\_\_\_\_

Searcher Location: \_\_\_\_\_

Date Searcher Picked Up: \_\_\_\_\_

Date Completed: 3-12-07

Searcher Prep & Review Time: 60

Online Time: 67

Type of Search

\_\_\_\_ NA Sequence (#)

\_\_\_\_ AA Sequence (#)

2 Structure (#)

\_\_\_\_ Bibliographic

\_\_\_\_ Litigation

\_\_\_\_ Fulltext

\_\_\_\_ Other

Vendors and cost where applicable

1030 STN \_\_\_\_\_ Dialog

\_\_\_\_ Questel/Orbit \_\_\_\_\_ Lexis/Nexis

\_\_\_\_ Westlaw \_\_\_\_\_ WWW/Internet

\_\_\_\_ In-house sequence systems

\_\_\_\_ Commercial \_\_\_\_\_ Oligomer \_\_\_\_\_ Score/Length

\_\_\_\_ Interference \_\_\_\_\_ SPDI \_\_\_\_\_ Encode/Transl

\_\_\_\_ Other (specify)

## INVENTOR SEARCH

=> fil capl; d ibib ed abs hitstr  
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FILE COVERS 1907 - 12 Mar 2007 VOL 146 ISS 12  
 FILE LAST UPDATED: 11 Mar 2007 (20070311/ED)

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 'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

*Search #1*

L20 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2003:855927 CAPLUS Full-text  
 DOCUMENT NUMBER: 139:350580  
 TITLE: Preparation of xanthinethione derivatives as myeloperoxidase inhibitors  
 INVENTOR(S): Hanson, Sverker; Nordvall, Gunnar; Tiden, Anna-Karin  
 PATENT ASSIGNEE(S): Astrazeneca AB, Swed.  
 SOURCE: PCT Int. Appl., 55 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003089430	A1	20031030	WO 2003-SE617	20030415
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2480452	A1	20031030	CA 2003-2480452	20030415
AU 2003224548	A1	20031103	AU 2003-224548	20030415
EP 1499613	A1	20050126	EP 2003-721211	20030415

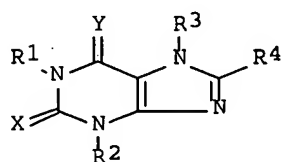
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

BR 2003009012	A	20050201	BR 2003-9012	20030415
CN 1646531	A	20050727	CN 2003-808355	20030415
JP 2005526836	T	20050908	JP 2003-586151	20030415
NZ 535406	A	20060831	NZ 2003-535406	20030415
ZA 2004007815	A	20051004	ZA 2004-7815	20040928
US 2005234036	A1	20051020	US 2004-511537	20041015 <--
NO 2004004998	A	20050118	NO 2004-4998	20041117
PRIORITY APPLN. INFO.:			SE 2002-1193	A 20020419
			SE 2002-2239	A 20020717
			WO 2003-SE617	W 20030415

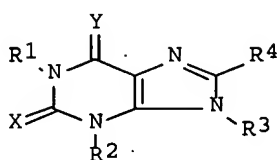
OTHER SOURCE(S): MARPAT 139:350580

ED Entered STN: 31 Oct 2003

GI



I



II

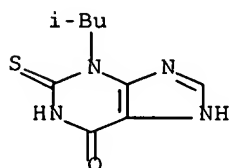
AB Xanthinethiones I and II [one of X and Y = S, the other = O, S; R1, R3, R4 = H, alkyl; R2 = H, (un)substituted alkyl] were prepared for use as myeloperoxidase (MPO) inhibitors in the treatment of neuroinflammatory disorders. Thus, Me2CHCH2NHCSNH2 was cyclized with NCCH2CO2Et to give 6-amino-1-isobutyl-2-thioxo-2,3-dihydro-1H-pyrimidin-4-one which was nitrosated, reduced to the 5,6-diamine, and cyclized with HCO2H to give II [R1, R3, R4 = H, R2 = CH2CHMe2, X = S, Y = O]. This compound had IC50 for inhibition of MPO of 0.87  $\mu$ M.

IT 618913-16-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of xanthinethione derivs. as myeloperoxidase inhibitors)

RN 618913-16-9 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-(2-methylpropyl)-2-thioxo- (9CI) (CA INDEX NAME)



IT 139460-82-5P 618913-20-5P 618913-24-9P  
618913-25-0P 618913-26-1P 618913-27-2P  
618913-28-3P

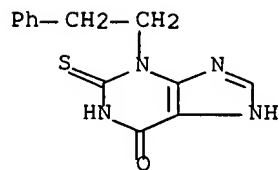
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)

(preparation of xanthinethione derivs. as myeloperoxidase inhibitors)

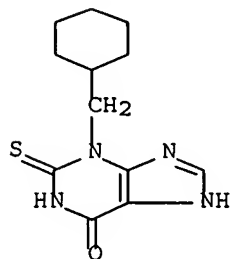
RN 139460-82-5 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-(2-phenylethyl)-2-thioxo- (9CI) (CA INDEX NAME)



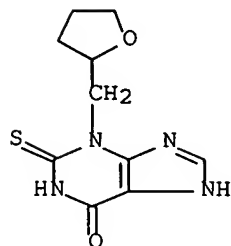
RN 618913-20-5 CAPLUS

CN 6H-Purin-6-one, 3-(cyclohexylmethyl)-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



RN 618913-24-9 CAPLUS

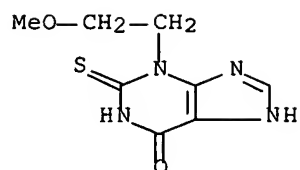
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-[(tetrahydro-2-furanyl)methyl]-2-thioxo- (9CI) (CA INDEX NAME)



RN 618913-25-0 CAPLUS

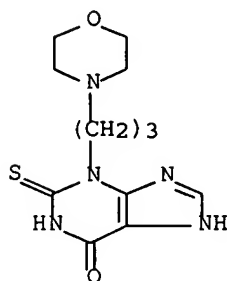
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-(2-methoxyethyl)-2-thioxo- (9CI) (CA INDEX NAME)





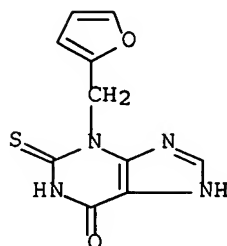
RN 618913-26-1 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-[3-(4-morpholinyl)propyl]-2-thioxo-  
(9CI) (CA INDEX NAME)



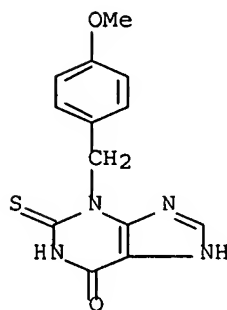
RN 618913-27-2 CAPLUS

CN 6H-Purin-6-one, 3-(2-furanylmethyl)-1,2,3,7-tetrahydro-2-thioxo- (9CI)  
(CA INDEX NAME)



RN 618913-28-3 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-[(4-methoxyphenyl)methyl]-2-thioxo-  
(9CI) (CA INDEX NAME)



IT 618913-30-7P 618913-31-8P

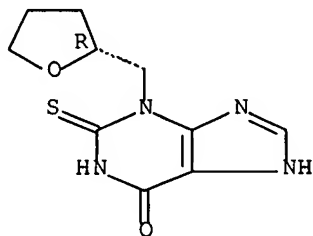
RL: PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of xanthinethione derivs. as myeloperoxidase inhibitors)

RN 618913-30-7 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-[[ (2R)-tetrahydro-2-furanyl]methyl]-2-thioxo- (9CI) (CA INDEX NAME)

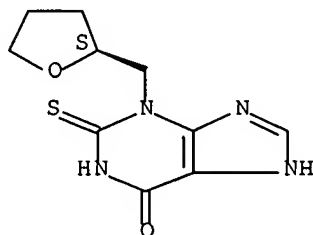
Absolute stereochemistry.



RN 618913-31-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-[[ (2S)-tetrahydro-2-furanyl]methyl]-2-thioxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 618913-11-4P 618913-12-5P 618913-13-6P

618913-14-7P 618913-15-8P 618913-17-0P

618913-18-1P 618913-21-6P 618913-22-7P

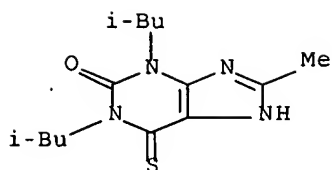
618913-23-8P 618913-29-4P 618913-32-9P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of xanthinethione derivs. as myeloperoxidase inhibitors)

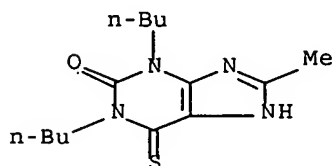
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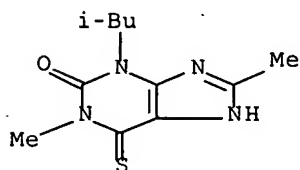
RN 618913-12-5 CAPLUS

CN 2H-Purin-2-one, 1,3-dibutyl-1,3,6,7-tetrahydro-8-methyl-6-thioxo- (9CI)  
(CA INDEX NAME)



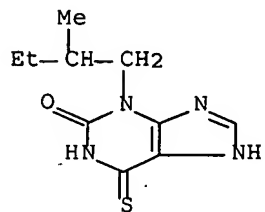
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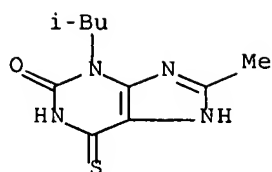
RN 618913-14-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(2-methylbutyl)-6-thioxo- (9CI) (CA INDEX NAME)



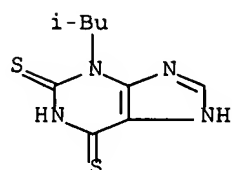
RN 618913-15-8 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-8-methyl-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



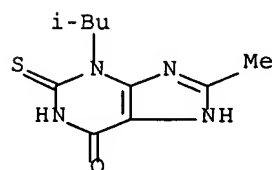
RN 618913-17-0 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-(2-methylpropyl)- (9CI) (CA INDEX NAME)



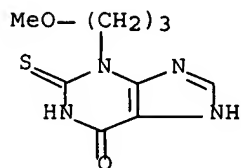
RN 618913-18-1 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-8-methyl-3-(2-methylpropyl)-2-thioxo- (9CI) (CA INDEX NAME)



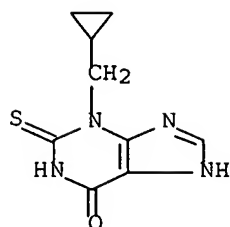
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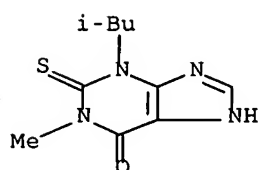
RN 618913-22-7 CAPLUS

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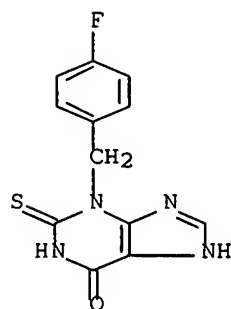
RN 618913-23-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1-methyl-3-(2-methylpropyl)-2-thioxo- (9CI) (CA INDEX NAME)



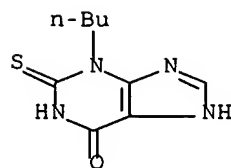
RN 618913-29-4 CAPLUS

CN 6H-Purin-6-one, 3-[(4-fluorophenyl)methyl]-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



RN 618913-32-9 CAPLUS

CN 6H-Purin-6-one, 3-butyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

7

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

## STRUCTURE SEARCH

=> fil reg; d stat que 17

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STRUCTURE FILE UPDATES: 11 MAR 2007 HIGHEST RN 926007-42-3

DICTIONARY FILE UPDATES: 11 MAR 2007 HIGHEST RN 926007-42-3

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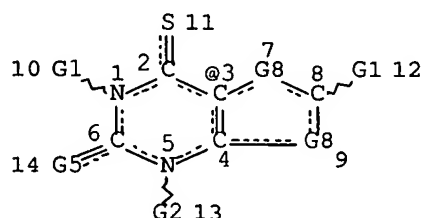
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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<http://www.cas.org/ONLINE/UG/regprops.html>

L4 STR

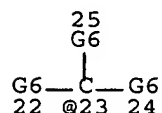


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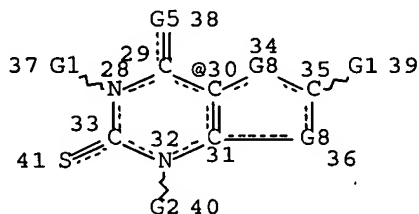
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O @27



G7 42

C @43

N-Ak  
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VAR G1=H/16

VAR G2=H/ME/17/20/23

VAR G5=O/S

VAR G6=27/43

VAR G7=3/30

VAR G8=15/NH/44

NODE ATTRIBUTES:

NSPEC IS RC AT 27  
NSPEC IS RC AT 43  
CONNECT IS X3 RC AT 8  
CONNECT IS E2 RC AT 15  
CONNECT IS E1 RC AT 16  
CONNECT IS X3 RC AT 35  
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DEFAULT MLEVEL IS ATOM  
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## GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 44

## STEREO ATTRIBUTES: NONE

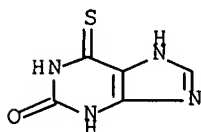
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3 REGISTRY NUMBERS YIELDED ~200 REFERENCES.  
ONLY THE OLDEST 5 PATENTS FOR EACH PROVIDED HERE.

=> d ide l10

L10 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 2002-59-7 REGISTRY  
ED Entered STN: 16 Nov 1984  
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-6-thioxo- (9CI)  
CN Xanthine, 6-thio- (6CI, 7CI, 8CI)  
OTHER NAMES:  
CN 2-Hydroxy-6-mercaptapurine  
CN 2-Hydroxy-6-thiopurine  
CN 3,6-Dihydro-6-thioxo-9H-purine-2(1H)-one  
CN 6-Mercaptoxanthine  
CN 6-Thioxanthine  
CN NSC 12160  
DR 3782-88-5  
MF C5 H4 N4 O S  
CI COM  
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN\*, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CSCHEM, DDFU, DRUGU, EMBASE, MEDLINE, PROMT, TOXCENTER, USPAT2, USPATFULL  
(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

192 REFERENCES IN FILE CA (1907 TO DATE)  
4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
192 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
23 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> fil capl; s l10

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FILE LAST UPDATED: 11 Mar 2007 (20070311/ED)

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'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

L41 192 L10

=> => d ibib ed abs hitstr 20-24

L43 ANSWER 20 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1992:230222 CAPLUS Full-text  
DOCUMENT NUMBER: 116:230222  
TITLE: Photodynamic tetrapyrrole inducer defoliants and herbicides. Porphyrin-heme biosynthesis modulator insecticides.  
INVENTOR(S): Rebeiz, Constantin A.  
PATENT ASSIGNEE(S): University of Illinois, USA  
SOURCE: PCT Int. Appl., 124 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 4  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9116820	A1	19911114	WO 1991-US3015	19910502
W: CA, JP, KR				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
US 5163990	A	19921117	US 1990-521119	19900503
US 5242892	A	19930907	US 1990-615413	19901119
EP 527186	A1	19930217	EP 1991-909022	19910502
R: BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL				
JP 06500989	T	19940127	JP 1991-508902	19910502
PRIORITY APPLN. INFO.:			US 1990-521119	A 19900503
			US 1990-615413	A 19901119
			US 1984-634932	B2 19840727
			US 1985-754092	B1 19850715
			US 1986-895529	A2 19860811
			WO 1991-US3015	W 19910502

ED Entered STN: 13 Jun 1992

AB A composition, which induces accumulation of photodynamic tetrapyrroles in the foliage of plants, comprises a chlorophyll biosynthesis modulator, optionally in combination with  $\delta$ -aminolevulinic acid. The composition is a herbicide, defoliant, or desiccant. An insecticidal composition which elevates endogenous tetrapyrrole levels in insects, comprises a porphyrin-heme biosynthesis modulator, optionally in combination with  $\delta$ -aminolevulinic acid. Thus, application of a combination containing 20 mM  $\delta$ -aminolevulinic acid and 15 mM 6-aminonicotinamide (modulator) defoliated tomato.

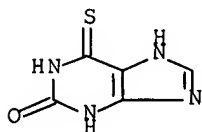
IT 2002-59-7

RL: BIOL (Biological study)

(photodynamic chlorophyll biosynthesis modulator, as plant controlling

agent)

RN 2002-59-7 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



L43 ANSWER 21 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1977:5495 CAPLUS Full-text  
 DOCUMENT NUMBER: 86:5495  
 TITLE: 2-Hydroxy-6-mercaptopurine  
 INVENTOR(S): Enoki, Kichiji; Genda, Yoshikazu; Hinoki, Yoshiaki  
 PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 51076294	A	19760701	JP 1975-3162	19741226
PRIORITY APPLN. INFO.:			JP 1975-3162	A 19741226

ED Entered STN: 12 May 1984

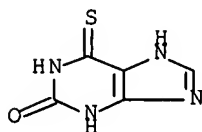
AB 2-Hydroxy-6-mercaptopurine (I) was prepared by heating 4(5)-thiocarbamoylimidazole-5(4)-carbamic acid esters in organic solvents. Thus, 5 g Me 4(5)-thiocarbamoylimidazole-5(4)-carbamate in DMF was stirred 2 hr at 140-50° to give 93% I.

IT 2002-59-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 2002-59-7 CAPLUS

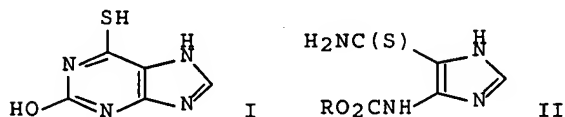
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



L43 ANSWER 22 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1976:433086 CAPLUS Full-text  
 DOCUMENT NUMBER: 85:33086  
 TITLE: 2-Hydroxy-6-mercaptopurine  
 INVENTOR(S): Enoki, Kichiji; Tomita, Nobuo; Genda, Yoshikazu;  
 Fukui, Takeo  
 PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 51008293	A	19760123	JP 1974-80779	19740716
PRIORITY APPLN. INFO.:			JP 1974-80779	A 19740716
ED Entered STN: 12 May 1984				
GI				



AB 2-Hydroxy-6-mercaptapurine (I) is prepared by cyclizing 4(5)-thiocarbamoylimidazole-5(4)-carbamate esters, e.g., II, with alkali or alcoholate in H<sub>2</sub>O or alcs. Thus, 2 g II (R = Me) was heated with 0.2 g NaOH in 20 ml H<sub>2</sub>O at 80-5° 3 hr to give 92.8% I. The yield was raised to 95.2% with 2 g NaOH or with 0.2 g Na in MeOH as the base.

IT 2002-59-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 2002-59-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



L43 ANSWER 23 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:433012 CAPLUS Full-text

DOCUMENT NUMBER: 85:33012

TITLE: 4(5)-Thiocarbamoylimidazole-5(4)-carbamate esters

INVENTOR(S): Enoki, Kichiji; Genda, Yoshikazu; Tomita, Nobuo; Fukui, Takeo

PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.  
 CODEN: JKXXAF

DOCUMENT TYPE: Patent

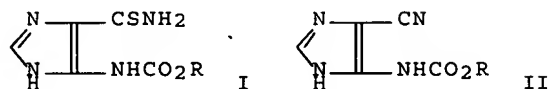
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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 JP 51008271      A      19760123      JP 1974-80778      19740716  
 PRIORITY APPLN. INFO.:      JP 1974-80778      A      19740716  
 ED Entered STN: 12 May 1984  
 GI



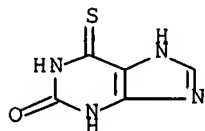
AB Title thioamides, e.g., I, are prepared by treating 4(5)-cyanoimidazole-5(4)-carbamate esters, e.g., II, with H<sub>2</sub>S in an organic solvent in the presence of aliphatic or alicyclic secondary amines. I are new compds. [substance claim] and are intermediates for 2-hydroxy-6-mercaptapurine (III). Thus, 8.3 g II (R = Me) and 0.1 g Et<sub>2</sub>NH in 50 ml DMF was treated with 3.3 g H<sub>2</sub>S at 50-5° 0.5 hr and heated 2 hr to give 90% I (R = Me). Iso-Bu<sub>2</sub>NH, piperidine, or pyrrolidine was also effective instead of Et<sub>2</sub>NH. Cyclization in 1% aqueous NaOH at 80-5° 3 hr gave 92.8% III.

IT 2002-59-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 2002-59-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



L43 ANSWER 24 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1969:78011 CAPLUS Full-text

DOCUMENT NUMBER: 70:78011

TITLE: 6-Thioxanthine

INVENTOR(S): Yamazaki, Satoshi; Meguro, Takashi; Kumashiro, Izumi

PATENT ASSIGNEE(S): Ajinomoto Co., Inc.

SOURCE: Jpn. Tokkyo Koho, 2 pp.

CODEN: JAXXAD

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 43006224	B4	19680307	JP	19651125

ED Entered STN: 12 May 1984

AB 5-Amino-4-thiocarbamoylimidazole (I) is heated with urea.. Thus, a mixture of 5 g. I and 10 g. urea is heated at 150-60° for 2 hrs., extracted with 0.5N NaOH, and the extract neutralized with AcOH to give 3.65 g. 6-thioxanthine. To prepare I, 50 g. 5-amino-4-carbamoylimidazole-HCl was mixed with 250 ml.

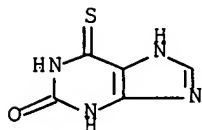
POCl<sub>3</sub> at 85° for 4 hrs. The mixture was cooled to give 19.6 g. 5-amino-4-cyanoimidazole (II), m. 128-9° (decomposition). A solution of 20 g. II in 360 ml. MeOH was mixed with 50 ml. KOH-MeOH solution (containing 155 g. KOH). The solution was saturated with H<sub>2</sub>S at room temperature, heated in a sealed tube at 100° for 2 hrs., and acidified with HOAc to give I.HOAc, which was dissolved in 2N HCl and the solution concentrated to give 15 g. I.HCl.

IT 2002-59-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 2002-59-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



=> fil reg; d ide l11

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DICTIONARY FILE UPDATES: 11 MAR 2007 HIGHEST RN 926007-42-3

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN

RN 2487-40-3 REGISTRY

ED Entered STN: 16 Nov 1984

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Xanthine, 2-thio- (6CI, 7CI, 8CI)

OTHER NAMES:

CN 2,3-Dihydro-2-thioxo-9H-purin-6(1H)-one

CN 2-Mercapto-6-hydroxypurine

CN 2-Mercaptohypoxanthine

CN 2-Thio-6-hydroxypurine

CN 2-Thioxanthine

CN 6-Hydroxy-2-mercaptapurine

CN 6-Hydroxypurine-2-thiol

CN NSC 36822

CN NSC 680828

DR 69-90-9, 3240-64-0, 5167-21-5, 6050-40-4

MF C5 H4 N4 O S

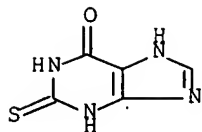
CI COM

LC STN Files: AGRICOLA, BEILSTEIN\*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, EMBASE, GMELIN\*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, PROMT, RTECS\*, TOXCENTER, USPAT2, USPATFULL

(\*File contains numerically searchable property data)

Other Sources: EINECS\*\*, NDSL\*\*, TSCA\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

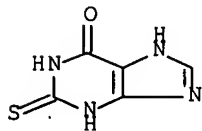
154 REFERENCES IN FILE CA (1907 TO DATE)  
 4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 154 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 20 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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L46 ANSWER 48 OF 52 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1969:524508 CAPLUS Full-text  
 DOCUMENT NUMBER: 71:124508  
 TITLE: 2-Mercaptopyrimidin-4(1H)-one  
 INVENTOR(S): Kawashima, Hideaki; Kumashiro, Izumi  
 PATENT ASSIGNEE(S): Ajinomoto Co., Inc.  
 SOURCE: Jpn. Tokkyo Koho, 2 pp.  
 CODEN: JAXXAD  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 44010790	B4	19690519	JP	19660211

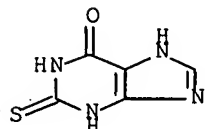
ED Entered STN: 12 May 1984  
 AB Manufacture of the title product (I) by heating 6-alkoxypurine 3-oxide (II) with an excess of thioacetic acid (III) is described. Thus, 1 g. II (alkyl = Me) in 20 ml. III is heated 4 hrs. at 98° to give 89% I, m. >360°.  
 IT 2487-40-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 2487-40-3 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



L46 ANSWER 49 OF 52 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1968:410477 CAPLUS Full-text  
 DOCUMENT NUMBER: 69:10477  
 TITLE: Purine derivatives

INVENTOR(S): Fujimoto, Yasuo; Teranishi, Masayuki  
 PATENT ASSIGNEE(S): Kyowa Fermentation Industry Co., Ltd.  
 SOURCE: Jpn. Tokkyo Koho, 7 pp.  
 CODEN: JAXXAD  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	JP 42020067	B4	19671006	JP	19640118
ED	Entered STN: 12 May 1984				
AB	2-(Phenylazocyno)acetamide (5.7 g.) and 7 g. formamidine acetate is refluxed 3 hrs. in 50 ml. Et Cellosolve, then a mixture of 20 ml. formamide and 2 to 4 g. Na hydrosulfite are added at 110-30° during 20 min., the mixture is kept at 110-30° for 30 min., then heated at 170-90° for 3 hrs., 200-300 ml. H <sub>2</sub> O added and filtered when hot, and the filtrate is treated with C, concentrated, and kept in a refrigerator overnight to give 2.4 g. hypoxanthine. Similarly prepared are 2-mercaptohypoxanthine, guanine, xanthine, 2-phenyl-6-hydroxypurine, 2-benzylhypoxanthine, 2-β-pyridyl-6-hydroxypurine, and 2-methyl-6-hydroxypurine.				
IT	2487-40-3P				
	RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)				
RN	2487-40-3 CAPLUS				
CN	6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)				



L46 ANSWER 50 OF 52 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1966:465567 CAPLUS Full-text  
 DOCUMENT NUMBER: 65:65567  
 ORIGINAL REFERENCE NO.: 65:12218f-g  
 TITLE: Preparation of purine and derivatives  
 PATENT ASSIGNEE(S): Kyowa Fermentation Industry Co., Ltd.  
 SOURCE: 7 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	FR 1425603		19660121	FR	
PRIORITY APPLN. INFO.:				JP	19640118
ED	Entered STN: 22 Apr. 2001				
AB	Derivs. of purine were prepared by treating an α-arylazocynoacetamide (I) with urea, thiourea, or an amidine. The condensation was followed by a catalytic or chemical reduction and a heating in the presence of a cyclizing agent such as formamide. Thus, a mixture of 5.7 parts 2-				



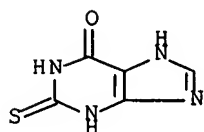
phenylazocycanoacetamide, 7 parts formamidine acetate, and 50 parts Et Cellosolve was boiled 3 hrs. then 20 parts formamide and 2.4 parts Na hydrosulfite added, and the mixture stirred 20 min. at 110-30° and 3 hrs. at 170-90°. Cooling, treating with 200-300 parts H<sub>2</sub>O, and filtering with C gave 2.4 parts free hypoxanthine. Similarly were prepared 2-mercaptohypoxanthine from ethyl 2-(p-hydroxyphenylazo)cycanoacetate and thiourea, guanine from ethyl 2-(p-methylphenylazo)cycanoacetate and guanidine carbonate, xanthine from ethyl 2-(m-phenylnitroazo)cycanoacetate and urea, 2-(methylthio)hypoxanthine from N-(2-phenylazocycanoacetyl)hydroxylamine and S-methylthiourea sulfate, and 2-methylhypoxanthine from 2-phenylazocycanoacetamide and acetamide-HCl.

IT 2487-40-3P, Xanthine, 2-thio-

RL: PREP (Preparation)  
(manufacture of)

RN 2487-40-3 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



L46 ANSWER 51 OF 52 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:27626 CAPLUS Full-text

DOCUMENT NUMBER: 64:27626

ORIGINAL REFERENCE NO.: 64:5116b-c

TITLE: Hypoxanthine

PATENT ASSIGNEE(S): Kyowa Fermentation Industry Co., Ltd.

SOURCE: 15 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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FR 1415149		19651022	FR 1964-995256	19641117
PRIORITY APPLN. INFO.:			JP	19631118

ED Entered STN: 22 Apr 2001

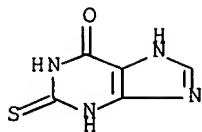
AB The title compound (I) was prepared by nitrosation of 4-amino-6-hydroxypyrimidine (II), reduction of the 5-nitroso compound, and ring closure in presence of HCONMe<sub>2</sub> (III) in one stage. Thus, II 11.1 was added to a mixture of NaNO<sub>2</sub> 7.3 and III 120, cooled to 0-4°, 98% HCO<sub>2</sub>H 7 added gradually, maintained at 10° for nitrosation, heated to 120-50°, Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub> added gradually within 10 min., refluxed at 180° for 1 hr., cooled, H<sub>2</sub>O added, and the precipitate filtered off to give 9.2 parts I.

IT 2487-40-3P, Xanthine, 2-thio-

RL: PREP (Preparation)  
(preparation of)

RN 2487-40-3 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



L46 ANSWER 52 OF 52 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1966:27625 CAPLUS Full-text  
 DOCUMENT NUMBER: 64:27625  
 ORIGINAL REFERENCE NO.: 64:5115h,5116a-b  
 TITLE: Purine derivatives  
 PATENT ASSIGNEE(S): Kyowa Fermentation Industry Co., Ltd.  
 SOURCE: 12 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1415224		19651022	FR 1964-996273	19641125
PRIORITY APPLN. INFO.:			JP	19631126

ED Entered STN: 22 Apr 2001

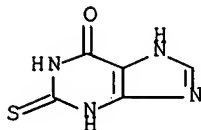
AB An improved process is reported for the reduction of o-aminoazopyrimidines and cyclization of the diamines produced to the aminopyrimidines. A cathode mixture containing 5.3 parts 4-amino-5-phenylazo-6-hydroxypyrimidine suspended in 150 vols. 50% HCO<sub>2</sub>H was electrolyzed for 2.5 hrs. using a Pb cathode (of area 27 cm.<sup>2</sup> per each 150 vols. of liquid) and a C anode, at a c.d. of 50-60 amp./dm.<sup>2</sup> at 90-105° until the initial color had disappeared. The resulting solution was refluxed for 8 hrs. to give 2.5 parts hypoxanthine (I). A similar reduction and cyclization was carried out in 3:1 90% HCO<sub>2</sub>H-HCONH<sub>2</sub>. Reduction and cyclization of 5.4 parts 4,6-diamino-5-phenylazopyrimidine similarly gave 2.7 parts adenine while 2,4-diamino-6-hydroxy-5-phenylazopyrimidine gave guanine. Other compds. prepared from the corresponding phenylazopyrimidines were (compound and % yield given): isoguanine, 81; 2,6-diaminopurine, 80; 2-aminopurine, 73; 2-diethylaminopurine, 75; 2-methylhypoxanthine, 75; 2-hydroxy-6-methylpurine, 71; 2-amino-6-methylpurine, 74; 2-mercaptioxanthine, 75; 2-mercapto-, 80, and 2-methylthioadenine, 79; 2-methylguanine 81; 1,3-diethylxanthine, 72.

IT 2487-40-3P, Xanthine, 2-thio-

RL: PREP (Preparation)  
 (preparation of)

RN 2487-40-3 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



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L12 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN

RN 5437-25-2 REGISTRY

ED Entered STN: 16 Nov 1984

CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1H-Purine-2,6-dithione, 3,7-dihydro- (9CI)

CN Xanthine, dithio- (6CI, 7CI, 8CI)

OTHER NAMES:

CN 2,6-Dimercaptopurine

CN 2,6-Dithiopurine

CN 2,6-Dithioxanthine

CN 2,6-Dithioxo-1,2,3,6-tetrahydro-9H-purine

CN Dithioxanthine

CN NSC 15989

CN NSC 685799

CN Purine-2,6-dithiol

DR 7390-61-6

MF C5 H4 N4 S2

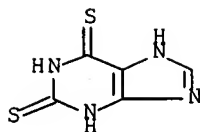
CI COM

LC STN Files: BEILSTEIN\*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CSCHEM, DDFU, DRUGU, IFICDB, IFIPAT, IFIUDB, MEDLINE, RTECS\*, TOXCENTER, USPAT2, USPATFULL

(\*File contains numerically searchable property data)

Other Sources: EINECS\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

90 REFERENCES IN FILE CA (1907 TO DATE)  
 90 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 12 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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L48 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1976:97840 CAPLUS Full-text  
 DOCUMENT NUMBER: 84:97840  
 TITLE: Photothermographic recording material  
 INVENTOR(S): White, Richard Lawson  
 PATENT ASSIGNEE(S): Eastman Kodak Co., USA  
 SOURCE: Ger. Offen., 32 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 2519585	A1	19751106	DE 1975-2519585	19750502
CA 1043617	A1	19781205	CA 1975-223845	19750429
BE 828685	A1	19751103	BE 1975-156028	19750502
FR 2269736	A1	19751128	FR 1975-13777	19750502
JP 50151138	A	19751204	JP 1975-52590	19750502
GB 1501005	A	19780215	GB 1975-18493	19750502
PRIORITY APPLN. INFO.:			US 1974-466331	A 19740502

ED Entered STN: 12 May 1984

AB Photothermog. recording materials giving images with a black tone and a high contrast are composed of a support having coated thereon a heat-developable, light-sensitive composition containing a Ag halide, a Ag salt of a heterocyclic thione, such as 3-carboxymethyl-4-methyl-4-thiazoline-2- thione Ag salt (I), an organic reducing agent, such as tert- butylhydroquinone, a heterocyclic mercapto compound as a toner, and a binder. Thus, an aqueous dispersion of I containing 9.6 mg Ag/ml 7, a 10% MeOH solution of tert- butylhydroquinone 1, a gelatin-AgI emulsion (21.2 mg Ag/ml and 0.06  $\mu$  average grain size) 0.4, nonylphenoxglycidol 0.4 ml, and 3-mercapto-1,2,4-triazole 1 mg were mixed, coated on a support, dried, imagewise exposed to unfiltered tungsten light, and developed from 2-8 sec at 160° to give an image d.  $\geq 1$ . The blue reflection d. and the visible reflection d. were then determined and their difference determined to be 0.12, which indicated that 3-mercapto-1,2,4-triazole was an especially good toner.

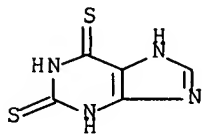
IT 5437-25-2

RL: USES (Uses)

(photothermog. copying compns. containing, for improved tone and contrast)

RN 5437-25-2 CAPLUS

CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



L48 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1975:18763 CAPLUS Full-text

DOCUMENT NUMBER: 82:18763

TITLE: Process and bath for increasing the polymer deposition velocity in electrolytic coating

INVENTOR(S): Dudley, Michael A.

PATENT ASSIGNEE(S): Canada Wire and Cable Co. Ltd.

SOURCE: Ger. Offen., 22 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	---	----	-----	-----
DE 2364936	A1	19740711	DE 1973-2364936	19731228
CA 976290	A1	19751014	CA 1972-160228	19721229
GB 1425389	A	19760218	GB 1973-58923	19731219
US 4020028	A	19770426	US 1974-429771	19740102
US 4136074	A	19790123	US 1975-630944	19751112
PRIORITY APPLN. INFO.:			CA 1972-160228	A 19721229
			US 1974-429771	A3 19740102

ED Entered STN: 12 May 1984

AB The rate of polymer deposition on a metal anode during electrophoretic coating with an epoxy ester, acrylic, or alkyd resin was increased by adding 0.01-2.0% Ac<sub>2</sub>CH<sub>2</sub> [123-54-6], 1H-1,2,4-triazole-3-thiol [3179-31-5], 3-mercapto-1,2-propanediol [96-27-5], 2-mercaptobenzoselenazole [10486-58-5], phenol [108-95-2], di(2-pyridyl)amine [1202-34-2], 2-mercaptopyrimidine [1450-85-7], or a similar compound to the baths. Thus, the rate of deposition of an epoxy ester resin on an Al anode was increased 70.6% by adding 0.2% Ac<sub>2</sub>CH<sub>2</sub> to the bath.

IT 5437-25-2

RL: USES (Uses)

(electrophoresis baths containing, for rapid coating)

RN 5437-25-2 CAPLUS

CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



L48 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1970:493614 CAPLUS Full-text  
 DOCUMENT NUMBER: 73:93614  
 TITLE: Use of silver pi-complex stabilizers  
 INVENTOR(S): Dunham, Kenneth R.  
 SOURCE: Def. Publ. U. S. Pat. Off. T, 22 pp. From: Off. Gaz.  
 1970, 877(3), 491.  
 CODEN: USXXBN  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 877011		19700818	US	19700211

ED Entered STN: 12 May 1984

AB A developed image in a photographic element containing a photographic  $\pi$ -complex of a Ag salt, especially a water-soluble salt and an organic compound, such as a Ag cycloheptatriene  $\pi$ -complex, can be stabilized with a Ag  $\pi$ -complex stabilizer, such as a thiadiazole, purine, benzimidazole, imidazoline, or pyrimidine. Such stabilizers are desirably odorless and form a stable Ag mercaptide. The photographic element can contain light-sensitive TiO<sub>2</sub>. An image in an exposed photographic element containing a photographic Ag  $\pi$ -complex, a Ag halide developing agent, and a Ag  $\pi$ -complex stabilizer can be developed and stabilized by heating the photographic element.

IT 5437-25-2  
 RL: USES (Uses)  
 (photographic processing solns. containing, for silver complex print-out emulsions)

RN 5437-25-2 CAPLUS

CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



L48 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1970:105870 CAPLUS Full-text  
 DOCUMENT NUMBER: 72:105870  
 TITLE: Development and stabilization of photographic films  
 INVENTOR(S): Cole, Roger M.  
 PATENT ASSIGNEE(S): Eastman Kodak Co.  
 SOURCE: Ger. Offen., 28 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1923824	A	19691211	DE 1969-1923824	19690509

US 3615511	A	19711026	US 1968-731275	19680522
FR 2009092	A5	19700130	FR 1969-16527	19690521
GB 1275074	A	19720524	GB 1969-1275074	19690522
PRIORITY APPLN. INFO.:			US 1968-731275	A 19680522

ED Entered STN: 12 May 1984

AB Fog formation during development or stabilization of imagewise exposed and optionally photodeveloped Ag halide recording materials of the internal image type can be avoided by use of developer solns. which are substantially free of strong Ag halide solvents and which contain, in addition to the usual developer compds. 1 + 10<sup>-5</sup>-2 + 10<sup>-3</sup> mole (1 + 10<sup>-5</sup>-4 + 10<sup>-3</sup> mole for use in conjunction with a process involving a Ag halide bleach solution) of a Ag complex forming compound which contains ≥1 group capable of undergoing covalent bond formation with Ag (e.g., a mercapto or imino group) and 1 group containing a π bond (e.g. the :I:C: bond). Stable images or copies are obtained with this type of developer solution (followed by fixation and washing) after exposure of print-out recording materials or after photodevelopment of direct copying photographic recording materials. Thus, several strips of a direct copying Ag halide emulsion were exposed (10<sup>-4</sup> sec, Xe lamp) through a step wedge and subsequently photodeveloped. The strips were developed (60 sec) in developer (A) containing H<sub>2</sub>O 800 ml, N-methyl-p-aminophenol sulfate 6, Na isoascorbate 40, KBr 1, K metabo rate 40, 4-methyl-1-phenyl-3-pyrazolidinone 1, 1-phenyl-5-mercaptotetrazole (I) 0.1 g, and H<sub>2</sub>O to 1 l., immersed (10 sec) in an AcOH stop bath, fixed (2 min) in a Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> solution, and washed (5 min) in running H<sub>2</sub>O and showed a background d. and image d. of 0.67 and 1.01, resp., vs. 0.48 and 0.46 for the control developed in I-free developer A. The presence of I in the developer solution prevented image reversal and enhanced the development of the highly exposed image areas. The resulting neg. image corresponded to that which would have been obtained by the customary photodevelopment used for direct copying recording materials.

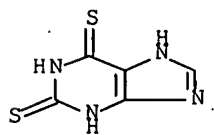
IT 5437-25-2

RL: USES (Uses)

(photographic developing solns. containing, for prevention of fog formation)

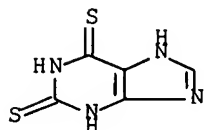
RN 5437-25-2 CAPLUS

CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



L48 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1969:524506 CAPLUS Full-text  
 DOCUMENT NUMBER: 71:124506  
 TITLE: 2,6- and 6,8-Dimercaptopurines  
 INVENTOR(S): Kawashima, Hideaki; Kumashiro, Izumi  
 PATENT ASSIGNEE(S): Ajinomoto Co., Inc.  
 SOURCE: Jpn. Tokkyo Koho, 2 pp.  
 CODEN: JAXXAD  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	JP 44010789	B4	19690516	JP	19660210
ED	Entered STN: 12 May 1984				
AB	Heating 6-chloropurine 3-oxide (I) with an excess of thioacetic acid (II) is described. Thus, 1 g. I is heated 6 hrs. at 98° with 25 g. II, the resulting yellow powder dissolved in dilute NH <sub>4</sub> OH and passed through a column of 300 ml. Dowex 50W-X4, and the column eluted with H <sub>2</sub> O and then with N NH <sub>4</sub> OH to give 14% 6,8-dimercaptopurine and 51% 2,6- dimercaptapurine, successively.				
IT	5437-25-2P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)				
RN	5437-25-2 CAPLUS				
CN	1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)				





## REFERENCES FOR ALL THE OTHER HITS

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 DICTIONARY FILE UPDATES: 11 MAR 2007 HIGHEST RN 926007-42-3

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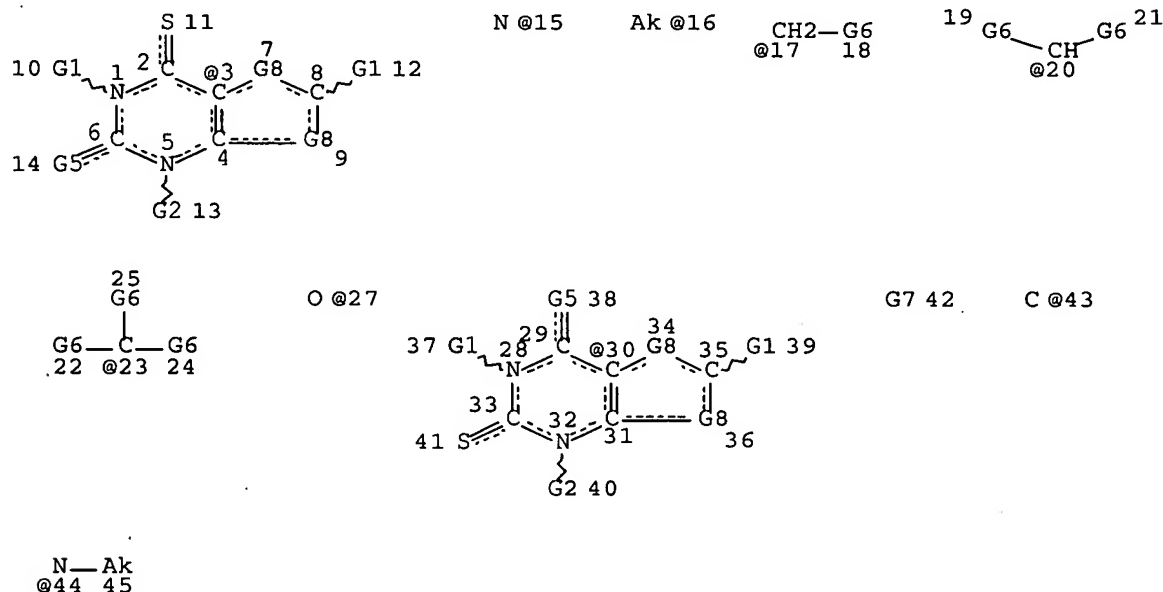
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L4

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 VAR G2=H/ME/17/20/23  
 VAR G5=O/S  
 VAR G6=27/43  
 VAR G7=3/30  
 VAR G8=15/NH/44

## NODE ATTRIBUTES:

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 NSPEC IS RC AT 43  
 CONNECT IS X3 RC AT 8  
 CONNECT IS E2 RC AT 15  
 CONNECT IS E1 RC AT 16  
 CONNECT IS X3 RC AT 35  
 CONNECT IS E1 RC AT 45  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

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 NUMBER OF NODES IS 44

## STEREO ATTRIBUTES: NONE

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 L8 444 SEA FILE=CAPLUS ABB=ON L7  
 L10 1 SEA FILE=REGISTRY ABB=ON 2002-59-7  
 L11 1 SEA FILE=REGISTRY ABB=ON 2487-40-3  
 L12 1 SEA FILE=REGISTRY ABB=ON 5437-25-2  
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 L14 122 SEA FILE=CAPLUS ABB=ON L13  
 L15 410 SEA FILE=CAPLUS ABB=ON L8 AND (PY<2003 OR AY<2003 OR PRY<2003)

L16 117 SEA FILE=CAPLUS ABB=ON L14 AND L15

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L57 116 L16 NOT L17

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L57 ANSWER 1 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:706960 CAPLUS Full-text

DOCUMENT NUMBER: 139:230796

TITLE: Synthesis of new purine derivatives

INVENTOR(S): Miyamoto, Kenichi; Sawanishi, Hiroyuki; Suzuki, Koichi; Yamamoto, Manabu; Shimura, Susumu

PATENT ASSIGNEE(S): Lotte Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

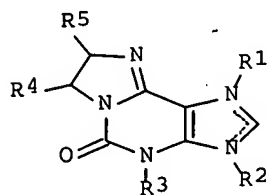
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003252875	A	20030910	JP 2002-58098	20020304 <--
KR 2003072251	A	20030913	KR 2003-13401	20030304 <--
PRIORITY APPLN. INFO.:			JP 2002-58098	A 20020304 <--

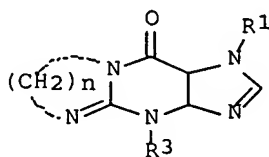
OTHER SOURCE(S): MARPAT 139:230796

ED Entered STN: 10 Sep 2003

GI



I



II

AB The patent relates to the preparation of purine derivs. and salts for pharmaceutical uses such as PDE IV isoenzyme inhibitor. The purine derivs. have the following formula (I) wherein R1, R2, R3 are hydrogen, or hydroxy, low alkyloxy, acyl substituted C1-C6 alkyl, or phenyl; and R4, and R5 are independently hydroxy, low alkyloxy, acyl substituted C1-C6 alkyl, or Ph group; and pharmaceutically compatible salts. The purine derivs. and pharmaceutically compatible salts may have the following formula (II) wherein R1, R2 are hydrogen, or hydroxy, low alkyloxy, acyl substituted C1-C6 alkyl, or phenyl; and n = 2 or 3. Thus, 8-methyl-4-propyl-4,5,7,8-tetrahydro-1H-imidazole-[2,1,i]purine-5-one prepared from 6-[(2-hydroxy-1-methyl)ethyl]amino-3-propylpurine-2-one in presence of triethylamine, and methanesulfonyl chloride was evaluated for PDE I test and gave greater activity than the control using Denoufylline.

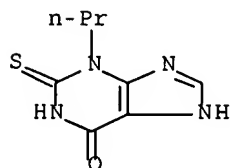
IT 156733-29-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in preparation of new purine derivs.)

RN 156733-29-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-propyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 2 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:723414 CAPLUS Full-text

DOCUMENT NUMBER: 138:137075

TITLE: Synthesis and cyclic AMP phosphodiesterase 4 isoenzyme inhibitory activity of heterocycle condensed purines

AUTHOR(S): Suzuki, Hirokazu; Yamamoto, Manabu; Shimura, Susumu; Miyamoto, Ken-ichi; Yamamoto, Kenji; Sawanishi, Hiroyuki

CORPORATE SOURCE: Department of Synthetic Chemistry, Hokuriku University, Kanazawa, 920-1181, Japan

SOURCE: Chemical &amp; Pharmaceutical Bulletin (2002), 50(9), 1163-1168

CODEN: CPBTAL; ISSN: 0009-2363

PUBLISHER: Pharmaceutical Society of Japan

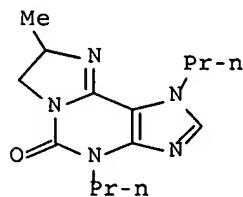
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:137075

ED Entered STN: 24 Sep 2002

GI



I

AB To reverse the adverse reactions of alkylxanthines and to develop novel inhibitors of cAMP phosphodiesterase 4 (PDE4), a series of heterocycle [a]-, [b]-, [c,d]-, and [i]-condensed purines were designed and synthesized. Although all compds. did not display PDE1 and PDE3 inhibitory activities, several heterocycle [i]-condensed purines strongly inhibited PDE4. Especially, dl-3,4-dipropyl-8-methyl-4,5,7,8-tetrahydro-1H-imidazo[2,1-i]purin-5-one (I) exhibited comparable PDE4 inhibitory activity (IC<sub>50</sub>=1.9 μM) to rolipram and denbufylline (DBF).

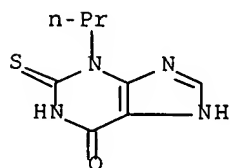
IT 156733-29-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heterocycle condensed purines from purine and pyrimidine  
derivs. and their activity as cAMP phosphodiesterase 4 isoenzyme  
inhibitors)

RN 156733-29-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-propyl-2-thioxo- (9CI) (CA INDEX  
NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 3 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:502824 CAPLUS Full-text

DOCUMENT NUMBER: 137:63122

TITLE: Preparation of purine derivatives or therapeutic use  
as phosphodiesterase IV inhibitors

INVENTOR(S): Chasin, Mark; Cavalla, David J.; Hofer, Peter; Gehrig,  
Andre; Wintergerst, Peter

PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg

SOURCE: U.S., 34 pp., Cont.-in-part of U.S. Ser. No. 285,473.  
CODEN: USXXAM

DOCUMENT TYPE: Patent

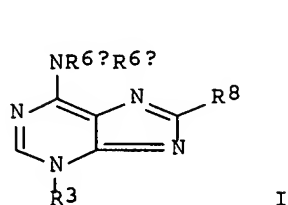
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 21

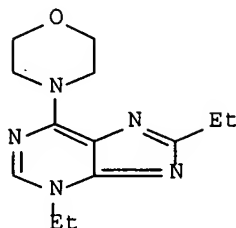
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6413975	B1	20020702	US 2000-539571	20000331 <--
IN 180930	A1	19980404	IN 1995-CA1508	19951123 <--
IN 181538	A1	19980711	IN 1995-CA1506	19951123 <--
HU 200200938	A2	20021028	HU 2002-938	20000331 <--
JP 2001316314	A	20011113	JP 2000-136383	20000509 <--
US 2003073834	A1	20030417	US 2002-62280	20020201 <--
PRIORITY APPLN. INFO.:			US 1999-285473	A2 19990402 <--
			IN 1994-CA514	A1 19940630 <--
			US 1997-963054	A2 19971103 <--
			US 1997-875487	A2 19971113 <--
			US 1998-151949	A2 19980911 <--
			US 1998-210556	A2 19981211 <--
			US 1998-210557	A2 19981211 <--
			US 1999-227057	A2 19990107 <--
			US 1999-237638	A2 19990126 <--
			US 1999-361196	A2 19990726 <--
			US 2000-506624	A2 20000218 <--
			US 2000-539571	A2 20000331 <--
			US 2000-547575	A2 20000412 <--
			US 2000-547898	A2 20000412 <--
			US 2000-636146	A2 20000810 <--
			US 2000-724321	B1 20001128 <--

OTHER SOURCE(S): MARPAT 137:63122  
 ED Entered STN: 04 Jul 2002  
 GI



I



II

AB Purines, such as I [R3, R6a, R6b, R8 = H, alkyl, alkenyl, cycloalkyl, aryl, arylalkyl, etc.], were prepared for pharmaceutical use as phosphodiesterase IV (PDE IV) inhibitors. Thus, 3,8-diethyl-6-morpholino-3H-purine (II) was prepared by conversion of 3,8-diethyl-2-thioxanthine to 3,8-diethylhypoxanthine using 2N NaOH and nickel aluminum alloy, reaction of 3,8-diethylhypoxanthine to 3,8-diethyl-6-thiohypoxanthine using phosphorus pentasulfide in pyridine and, finally, reaction of 3,8-diethyl-6-thiohypoxanthine with morpholine. The prepared purine derivs. were assayed for PDE IV inhibition.

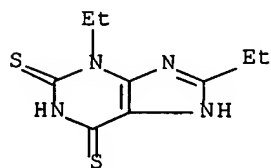
IT 162278-92-4P, 3,8-Diethyl-2,6-dithioxanthine 162279-04-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of purine derivs. for therapeutic use as phosphodiesterase IV inhibitors)

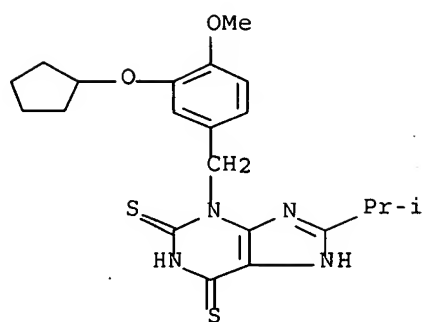
RN 162278-92-4 CAPLUS

CN 1H-Purine-2,6-dithione, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 162279-04-1 CAPLUS

CN 1H-Purine-2,6-dithione, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



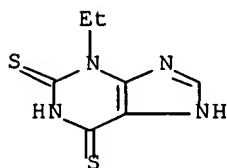
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 162279-08-5P 162279-09-6P 162279-10-9P  
 300783-48-6P 300783-53-3P 439694-45-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of purine derivs. for therapeutic use as phosphodiesterase IV  
 inhibitors)

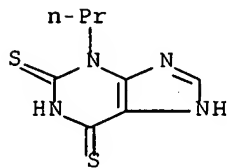
RN 162278-87-7 CAPLUS

CN 1H-Purine-2,6-dithione, 3-ethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



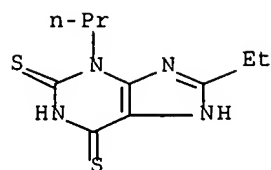
RN 162278-88-8 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-propyl- (9CI) (CA INDEX NAME)



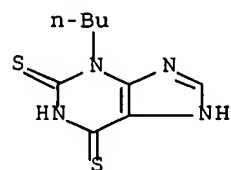
RN 162278-89-9 CAPLUS

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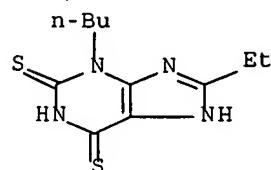
RN 162278-90-2 CAPLUS

CN 1H-Purine-2,6-dithione, 3-butyl-3,7-dihydro- (9CI) (CA INDEX NAME)



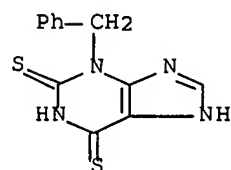
RN 162278-91-3 CAPLUS

CN 1H-Purine-2,6-dithione, 3-butyl-8-ethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 162278-93-5 CAPLUS

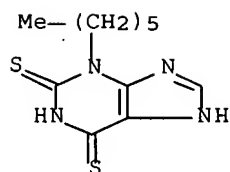
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 162278-94-6 CAPLUS

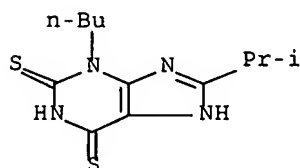
CN 1H-Purine-2,6-dithione, 3-hexyl-3,7-dihydro- (9CI) (CA INDEX NAME)





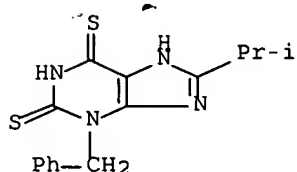
RN 162279-01-8 CAPLUS

CN 1H-Purine-2,6-dithione, 3-butyl-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



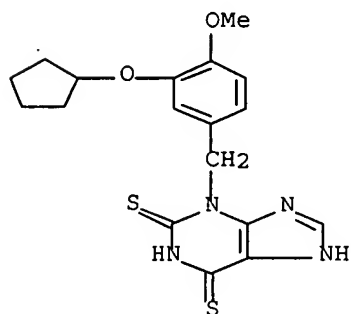
RN 162279-02-9 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



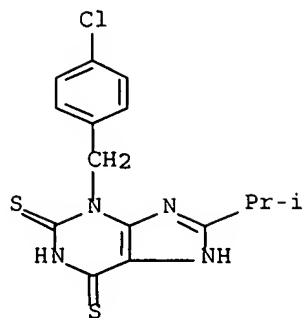
RN 162279-05-2 CAPLUS

CN 1H-Purine-2,6-dithione, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro- (9CI) (CA INDEX NAME)



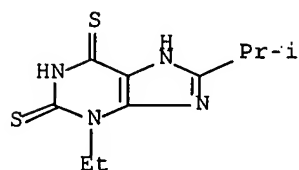
RN 162279-06-3 CAPLUS

CN 1H-Purine-2,6-dithione, 3-[(4-chlorophenyl)methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



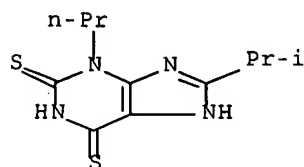
RN 162279-07-4 CAPLUS

CN 1H-Purine-2,6-dithione, 3-ethyl-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



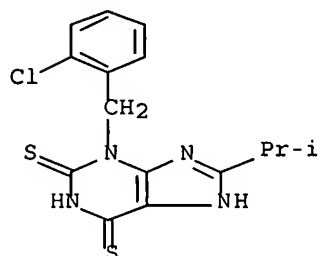
RN 162279-08-5 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-propyl- (9CI) (CA INDEX NAME)



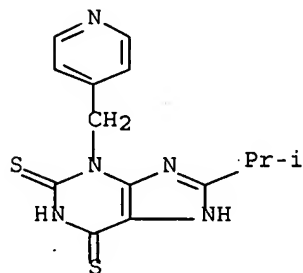
RN 162279-09-6 CAPLUS

CN 1H-Purine-2,6-dithione, 3-[(2-chlorophenyl)methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



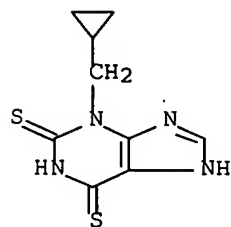
RN 162279-10-9 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



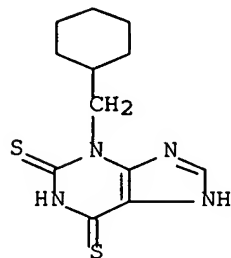
RN 300783-48-6 CAPLUS

CN 1H-Purine-2,6-dithione, 3-(cyclopropylmethyl)-3,7-dihydro- (9CI) (CA INDEX NAME)



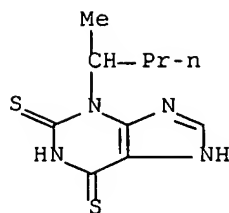
RN 300783-53-3 CAPLUS

CN 1H-Purine-2,6-dithione, 3-(cyclohexylmethyl)-3,7-dihydro- (9CI) (CA INDEX NAME)

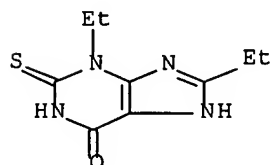


RN 439694-45-8 CAPLUS

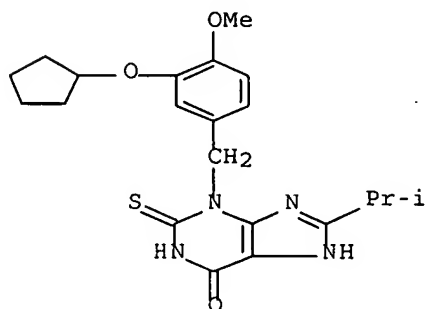
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-(1-methylbutyl)- (9CI) (CA INDEX NAME)



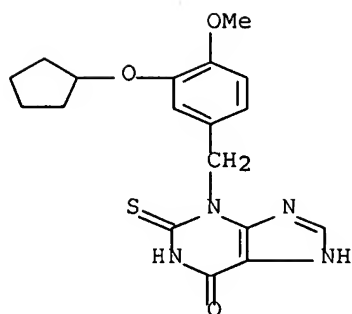
IT 162278-04-8, 3,8-Diethyl-2-thioxanthine  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of purine derivs. for therapeutic use as phosphodiesterase IV inhibitors)  
 RN 162278-04-8 CAPLUS  
 CN 6H-Purin-6-one, 3,8-diethyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



IT 300781-30-0P, 3-(3-Cyclopentyloxy-4-methoxybenzyl)-8-isopropyl-2-thioxanthine 300781-35-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of purine derivs. for therapeutic use as phosphodiesterase IV inhibitors)  
 RN 300781-30-0 CAPLUS  
 CN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,2,3,7-tetrahydro-8-(1-methylethyl)-2-thioxo- (9CI) (CA INDEX NAME)

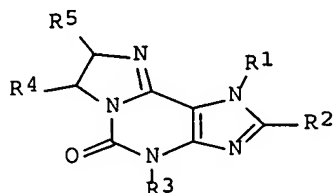


RN 300781-35-5 CAPLUS  
 CN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)

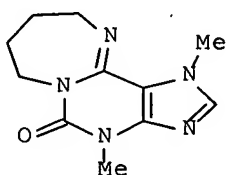


REFERENCE COUNT: 86 THERE ARE 86 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 4 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2002:485205 CAPLUS Full-text  
 DOCUMENT NUMBER: 137:201279  
 TITLE: Imidazo[2,1-i]purin-5-ones and Related Tricyclic Water-Soluble Purine Derivatives: Potent A2A- and A3-Adenosine Receptor Antagonists  
 AUTHOR(S): Mueller, Christa E.; Thorand, Mark; Qurishi, Ramatullah; Diekmann, Martina; Jacobson, Kenneth A.; Padgett, William L.; Daly, John W.  
 CORPORATE SOURCE: Pharmaceutical Institute Poppelsdorf, University of Bonn, Bonn, Germany  
 SOURCE: Journal of Medicinal Chemistry (2002), 45(16), 3440-3450  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 137:201279  
 ED Entered STN: 28 Jun 2002  
 GI



I



II

AB A series of tricyclic imidazo[2,1-i]purinones I [R1, R4 = H, Me; R2 = H, Ph, (E)-PhCH:CH; R3 = H, Me, PhCH2; R5 = H, Me, Et] and ring-enlarged analogs, e.g. II, derived from xanthine derivs. were prepared as adenosine receptor (AR) antagonists. In comparison with xanthines, these tricyclic compds. exhibited increased water solubility due to a basic nitrogen atom, which can be protonated under physiol. conditions. A new capillary electrophoresis method was developed for the determination of the enantiomeric purity of selected chiral products using native and modified  $\beta$ -cyclodextrins as chiral discriminators. The compds. were investigated in radioligand binding assays at rat brain A1 and A2A ARs. Selected I were addnl. investigated in

radioligand binding assays at human recombinant A3 ARs and in functional studies (adenylate cyclase assays) at A1 ARs of rat fat cell membranes, A2A ARs of rat PC 12 cell membranes, and mouse A2B ARs of NIH 3T3 cell membranes, and showed the structure-activity relationships similar to those of the corresponding xanthine derivs. The 2-styrylimidazopurinones I [R1 = H, Me; R2 = (E)-PhCH:CH; R3 = Me; R4 = H, R5 = Et] were less potent at A2A ARs as compared to 8-styrylxanthine derivs. The most potent compound at A2A ARs was (S)-I [R1 = R3 = Me, R2 = (E)-PhCH:CH, R4 = H, R5 = Et; (III)] exhibiting a Ki value of 424 nM at rat A2A ARs. III was also highly selective for A2A receptors vs A1 and A3 ARs; however, the selectivity vs A2B ARs was low. Among the 1-unsubstituted (2-phenyl)imidazopurinones, the most potent A3 antagonist was (R)-I (R1 = R4 = H, R2 = Ph, R3 = Me, R5 = Et) exhibiting a Ki value of 2.3 nM and high selectivity for A3 receptors vs all other AR subtypes.

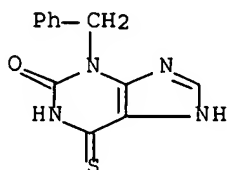
IT 19844-94-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of imidazopurinones and ring-enlarged analogs as adenosine receptor antagonists via thiation of xanthines, methylation of thioxopurinones, coupling of (methylthio)purinones with amino alcs., and heterocyclization)

RN 19844-94-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(phenylmethyl)-6-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 5 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:90055 CAPLUS Full-text

DOCUMENT NUMBER: 136:131252

TITLE: Cationic materials and methods for covalent bonding nucleic acids to high purity silica surfaces

INVENTOR(S): Lyles, Mark B.

PATENT ASSIGNEE(S): USA

SOURCE: PCT Int. Appl., 9 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008237	A2	20020131	WO 2001-US23079	20010720 <--
WO 2002008237	A3	20021107		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,

LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,  
 RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ,  
 VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
 BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2001076023 A5 20020205 AU 2001-76023 20010720 <--  
 US 2002103350 A1 20020801 US 2001-910697 20010720 <--  
 US 6855817 B2 20050215  
 EP 1305328 A2 20030502 EP 2001-953590 20010720 <--

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

US 2005148067 A1 20050707 US 2005-57440 20050214 <--

PRIORITY APPLN. INFO.:

US 2000-220096P P 20000721 <--  
 US 2001-910697 A 20010720 <--  
 WO 2001-US23079 W 20010720 <--

ED Entered STN: 01 Feb 2002

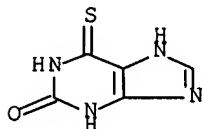
AB Surfaces containing high purity silica (silicon dioxide) exhibit high loading potential for nucleic acids. Formulations containing nucleic acids and materials which mask the electrostatic interactions between the nucleic acids and surfaces are disclosed. By masking the phosphate charges of the nucleic acids, undesired interactions may be minimized or eliminated, thereby allowing the covalent bonding of the nucleic acids to the surface to proceed. The use of such formulations addnl. minimizes nonspecific binding of the nucleic acids to the surface. Examples of materials to be included in such formulations include cations, xanthenes, hexoses, purines, arginine, lysine, polyarginine, polylysine, and quaternary ammonium salts.

IT 2002-59-7, 6-Thioxanthine 5437-25-2, 2,6-Dithiopurine  
 91725-06-3

RL: NUU (Other use, unclassified); USES (Uses)  
 (cationic materials and methods for covalent bonding nucleic acids to  
 high purity silica surfaces)

RN 2002-59-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



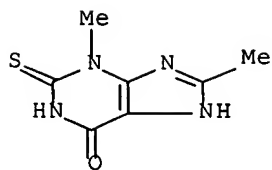
RN 5437-25-2 CAPLUS

CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



RN 91725-06-3 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3,8-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 6 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:413184 CAPLUS Full-text

DOCUMENT NUMBER: 135:251414

TITLE: Structural predictions of adenosine 2B antagonist affinity using molecular field analysis

AUTHOR(S): Song, Yuqing; Coupar, Ian M.; Iskander, Magdy N.

CORPORATE SOURCE: Department of Medicinal Chemistry, Victorian College of Pharmacy, Monash University, Parkville, 3052, Australia

SOURCE: Quantitative Structure-Activity Relationships (2001), 20(1), 23-30

CODEN: QSARDI; ISSN: 0931-8771

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 08 Jun 2001

AB 3D structural evaluation of the adenosine 2B (A2B) antagonist binding site is the major aim for developing specific selective antagonists. In an attempt to deduce structural properties of the antagonist site, a pharmacophore model was developed using 85 known A2B antagonists. The mol. mechanics optimization methods were used to deduce the likely binding conformations of the antagonists at the binding site. Super-imposition of the antagonists was carried out using fit-atoms. This alignment was used to develop CoMFA models of the A2B antagonist binding site. The models possessed promising predictive ability as indicated by the high cross-validated correlation ( $q^2 = 0.752$ ,  $r^2 = 0.982$ ) and the prediction on the external test set. The analyses showed that steric and electrostatic interactions contributed to A2B antagonist biol. activity equally. The hydrogen-bond donor nature of the 7-position of xanthine (1 .apprx. 68) and 3-position of alloxazine (83) was essential for the biol. activity. In addition, the presence of more neg. charges on the 1-N position of xanthine and 10-N position of alloxazine increases biol. activity. The bulky aromatic substitutions on the 8-position of xanthine compds. improve activity, while an alkyl substitution on the 1-position of alloxazine might enhance activity. The model generated from this investigation produced important structural requirements, which will be used to optimize the structural complementarity of the antagonists at the A2B binding site.

IT 2398-70-1, 6-Thiotheophylline 6603-63-0

42458-91-3, 1-Methyl-3-isobutyl-6-thioxanthine

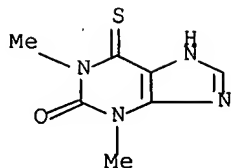
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(structural predictions of adenosine 2B antagonist affinity using mol. field anal.)

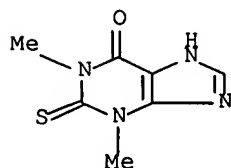
RN 2398-70-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)

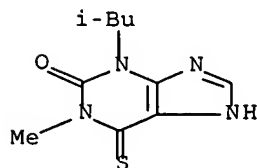




RN 6603-63-0 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 42458-91-3 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 7 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2001:413183 CAPLUS Full-text  
 DOCUMENT NUMBER: 135:164033  
 TITLE: An updated topographical model for phosphodiesterase 4 (PDE4) catalytic site  
 AUTHOR(S): Fossa, Paola; Menozzi, Giulia; Mosti, Luisa  
 CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Genoa, 16132, Italy  
 SOURCE: Quantitative Structure-Activity Relationships (2001), 20(1), 17-22  
 CODEN: QSARDI; ISSN: 0931-8771  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 08 Jun 2001  
 AB Preclin. and clin. studies on cyclic nucleotide phosphodiesterases 4 (PDE4) inhibitors showed that these agents might be employed in the treatment of allergic diseases, in particular asthma. Unfortunately, many of these compds.

such as rolipram, which belongs to the so-called first generation" showed undesirable side effects such as nausea and emesis. Efforts to eliminate these adverse side effects prompted the synthesis of a second generation of PDE4 inhibitors, with improved selectivity toward the enzyme catalytic site. So as to refine the pharmacophoric models of the catalytic site previously described in literature and better define the structural requirements which are essential for potent and selective PDE4 inhibition, we undertook the present computational study. DISCO approach was applied to generate an optimal alignment for a set of structurally diverse selective inhibitors 1-18 chosen from the literature. The resulting superimposition of common pharmacophoric elements was refined by evaluating mol. field properties. A rational pharmacophoric model of the enzyme active site was thus derived and tested for its ability in predicting the degree of potency for a novel ligand. The comparison of the pharmacophoric areas common to cAMP, the natural substrate of the enzyme, and the most selective inhibitors was performed so as to better understand the binding mode of PDE4 selective inhibitors in the catalytic site.

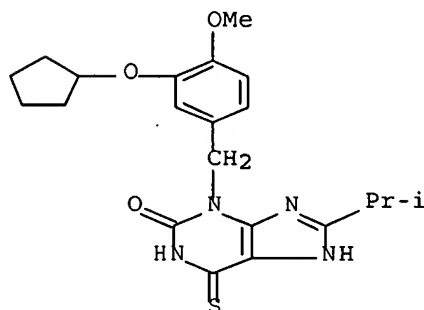
IT 179486-28-3

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)

(updated topog. model for phosphodiesterase 4 (PDE4) catalytic site)

RN 179486-28-3 CAPLUS

CN 2H-Purin-2-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 8 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:136945 CAPLUS Full-text

DOCUMENT NUMBER: 134:193441

TITLE: Preparation of hypoxanthines and thiohypoxanthines as phosphodiesterase IV inhibitors

INVENTOR(S): Chasin, Mark; Hofer, Peter; Cavalla, David

PATENT ASSIGNEE(S): Euro-Celtique S.A., Luxembourg

SOURCE: PCT Int. Appl., 68 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

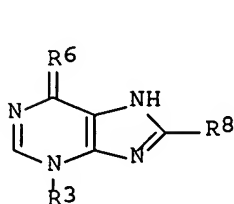
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

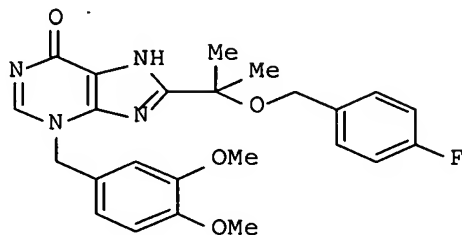
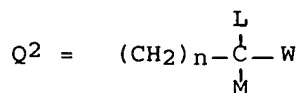
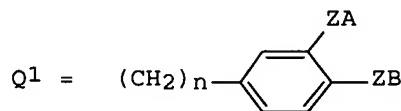
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2001011967      A1      20010222      WO 2000-US21836      20000809 <--  
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HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,  
LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,  
SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,  
YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,  
CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
CA 2379356      A1      20010222      CA 2000-2379356      20000809 <--  
EP 1202628      A1      20020508      EP 2000-953925      20000809 <--  
EP 1202628      B1      20041013  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL  
JP 2003506467      T      20030218      JP 2001-516330      20000809 <--  
AT 279113      T      20041015      AT 2000-953925      20000809 <--  
PRIORITY APPLN. INFO.:      US 1999-148623P      P 19990812 <--  
OTHER SOURCE(S):      MARPAT 134:193441      WO 2000-US21836      W 20000809 <--  
ED Entered STN: 25 Feb 2001  
GI



I



II

AB Title compds. (I) [wherein R3 and R8 = independently (cyclo)alkyl, alkenyl, alkynyl, Q1, or Q2; R6 = S or O; n = 0-1; Z = a bond, CH2, NH, O, or S; A and B can form a ring by adding 1-3 CH2 groups when Z = CH2, NH, O or S; and A and B are not in a ring when Z = a bond, wherein A and B = independently H, halo, (cyclo)alkyl, (cyclo)alkoxy, OH, or (un)substituted Ph, benzyl, or benzyloxy; L and M = independently H or Me; W = Q1, OH, (hetero)aryl, heterocyclyl, or (un)substituted benzyloxy] were prepared as selective phosphodiesterase (PDE) IV inhibitors. For example, amidation of 2-(4-fluorobenzyloxy)-2-methylpropionyl chloride with 5,6-diamino-1-(3,4-dimethoxybenzyl)-2-thiouracil using TEA in THF (20.4%), followed by cyclization with NaOH to form the 2-thioxanthine (79.1%) and treatment with Raney nickel in 1-propanol (67.2%), afforded the hypoxanthine (II). In assays measuring isolated PDE isoenzyme

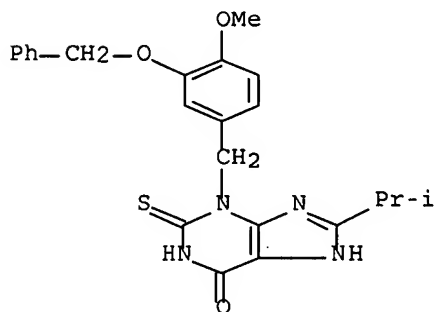
activity, II selectively inhibited PDE IV compared to PDE III and PDE V with IC50 values of 1.079  $\mu$ M, 69.62  $\mu$ M, and 35.80  $\mu$ M, resp. As a result, I are expected to induce the desirable anti-asthmatic effects associated with PDE IV inhibition without causing the undesirable cardiovascular stimulation associated with PDE III inhibition (no data). I are useful in the treatment of asthma, allergies, inflammation, depression, dementia, and other disease states associated with abnormally high physiolo. levels of cytokine (no data).

IT 227763-83-9P, 3-(3-Benzyloxy-4-methoxybenzyl)-8-isopropyl-2-thioxanthine 327036-65-7P, 3-(3,4-Methylenedioxybenzyl)-8-(1-methylethyl)-2-thioxanthine 327036-70-4P, 3-(3,4-Dimethoxybenzyl)-8-(1-methylethyl)-2-thioxanthine  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of hypoxanthine and thiohypoxanthine phosphodiesterase IV inhibitors from thiouracils and acyl halides and anhydrides)

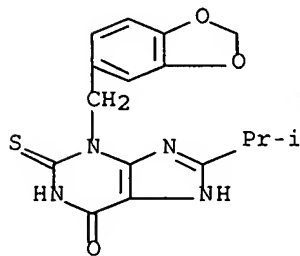
RN 227763-83-9 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-[[4-methoxy-3-(phenylmethoxy)phenyl]methyl]-8-(1-methylethyl)-2-thioxo- (9CI) (CA INDEX NAME)



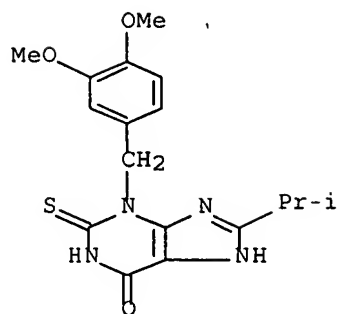
RN 327036-65-7 CAPLUS

CN 6H-Purin-6-one, 3-(1,3-benzodioxol-5-ylmethyl)-1,2,3,7-tetrahydro-8-(1-methylethyl)-2-thioxo- (9CI) (CA INDEX NAME)

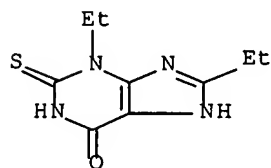


RN 327036-70-4 CAPLUS

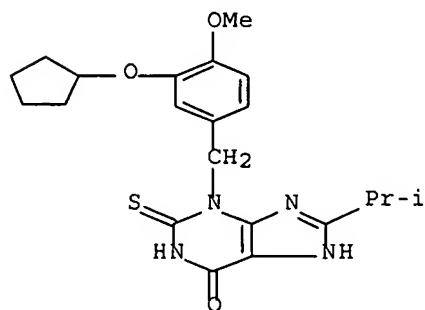
CN 6H-Purin-6-one, 3-[(3,4-dimethoxyphenyl)methyl]-1,2,3,7-tetrahydro-8-(1-methylethyl)-2-thioxo- (9CI) (CA INDEX NAME)



IT 162278-04-8, 3,8-Diethyl-2-thioxanthine 300781-30-0,  
 3-(3-Cyclopentyloxy-4-methoxybenzyl)-8-isopropyl-2-thioxanthine  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (starting material; preparation of hypoxanthine and thiohypoxanthine  
 phosphodiesterase IV inhibitors from thiouracils and acyl halides and  
 anhydrides)  
 RN 162278-04-8 CAPLUS  
 CN 6H-Purin-6-one, 3,8-diethyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX  
 NAME)



RN 300781-30-0 CAPLUS  
 CN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,2,3,7-  
 tetrahydro-8-(1-methylethyl)-2-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 9 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2000:725418 CAPLUS Full-text  
 DOCUMENT NUMBER: 133:296324  
 TITLE: Synthesis and phosphodiesterase IV inhibition activity

of purine derivatives

INVENTOR(S): Chasin, Mark; Cavalla, David; Hofer, Peter; Gehrig, Andre; Wintergest, Peter

PATENT ASSIGNEE(S): Euro-Celtique S.A., Luxembourg

SOURCE: PCT Int. Appl., 112 pp.  
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 21

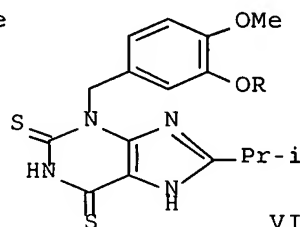
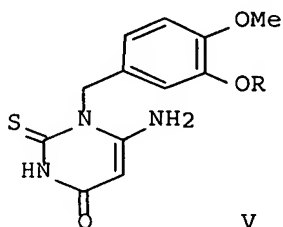
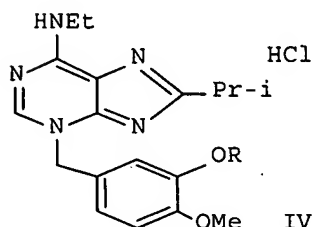
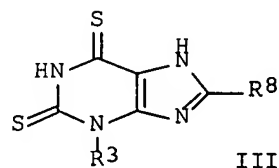
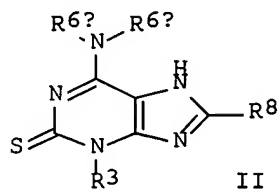
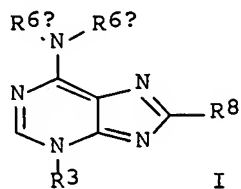
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000059449	A2	20001012	WO 2000-US8525	20000331 <--
WO 2000059449	A3	20010104		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
IN 180930	A1	19980404	IN 1995-CA1508	19951123 <--
IN 181538	A1	19980711	IN 1995-CA1506	19951123 <--
CA 2367143	A1	20001012	CA 2000-2367143	20000331 <--
EP 1169321	A2	20020109	EP 2000-919929	20000331 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
HU 200200938	A2	20021028	HU 2002-938	20000331 <--
JP 2002541078	T	20021203	JP 2000-609014	20000331 <--
BR 2000011182	A	20030610	BR 2000-11182	20000331 <--
JP 2001316314	A	20011113	JP 2000-136383	20000509 <--
PRIORITY APPLN. INFO.:				
			US 1999-285473	A 19990402 <--
			IN 1994-CA514	A1 19940630 <--
			WO 2000-US8525	W 20000331 <--

OTHER SOURCE(S): MARPAT 133:296324

ED Entered STN: 13 Oct 2000

GI



AB The purine (I) (R3, R8, R6a, R6b = H, (un)substituted alkyl, alkenyl, cycloalkyl, aryl, heterocyclyl, heteroaryl etc.), thioisoguanine (II), dithioxanthine (III) derivs., and their pharmaceutically accepted salts were synthesized. Thus, purine (IV; R = (CH<sub>2</sub>)<sub>5</sub>) was prepared by etherification of isovanilline with cyclopentanol, oximation, reduction to amine, conversion to isothiocyanate, amination to thiourea followed by heterocyclization with Et cyanoacetate to thiouracil (V). V was nitrosylated, reduced, reacted with isobutyric anhydride to give isobutyrylamine which on treatment with phosphorus pentasulfide gave dithioxanthine (VI). VI, in a pressure reactor gave purine-2-thione which was reduced with Raney-nickel to give IV. The IC<sub>50</sub> of IV against phosphodiesterase IV inhibition was 0.32  $\mu$ M. I, II and III were effective in effecting PDE IV inhibition in patients in need thereof.

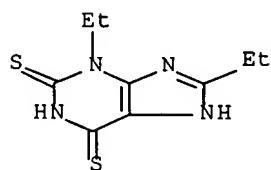
IT 162278-92-4P, 3,8-Diethyl-2,6-dithioxanthine 162279-04-1P  
162279-05-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of purine derivs. as phosphodiesterase IV inhibitors)

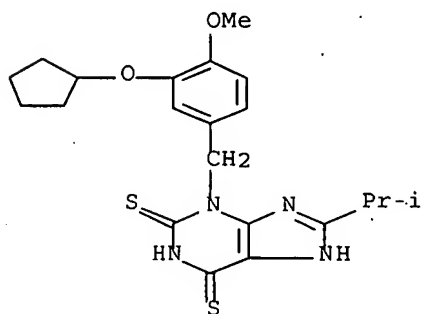
RN 162278-92-4 CAPLUS

CN 1H-Purine-2,6-dithione, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



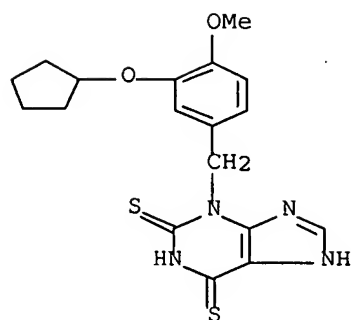
RN 162279-04-1 CAPLUS

CN 1H-Purine-2,6-dithione, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 162279-05-2 CAPLUS

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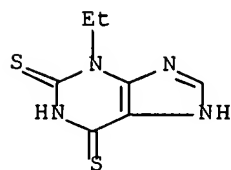


IT 162278-87-7P 162278-88-8P 162278-89-9P  
 162278-90-2P 162278-91-3P 162278-93-5P  
 162278-94-6P 162279-01-8P 162279-02-9P  
 162279-06-3P 162279-07-4P 162279-08-5P  
 162279-09-6P 162279-10-9P 300783-45-3P  
 300783-48-6P 300783-53-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of purine derivs. as phosphodiesterase IV inhibitors)

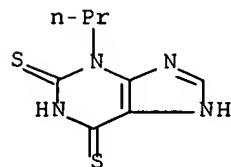
RN 162278-87-7 CAPLUS

CN 1H-Purine-2,6-dithione, 3-ethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 162278-88-8 CAPLUS

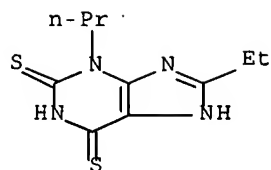
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-propyl- (9CI) (CA INDEX NAME)



RN 162278-89-9 CAPLUS

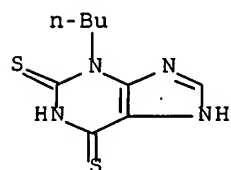
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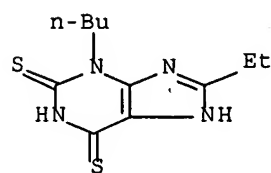
RN 162278-90-2 CAPLUS

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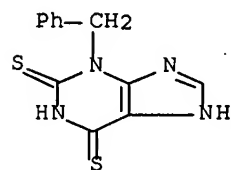
RN 162278-91-3 CAPLUS

CN 1H-Purine-2,6-dithione, 3-butyl-8-ethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



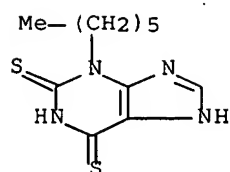
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CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



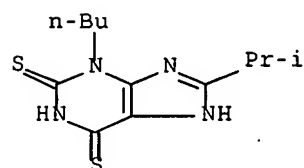
RN 162278-94-6 CAPLUS

CN 1H-Purine-2,6-dithione, 3-hexyl-3,7-dihydro- (9CI) (CA INDEX NAME)



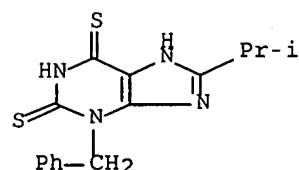
RN 162279-01-8 CAPLUS

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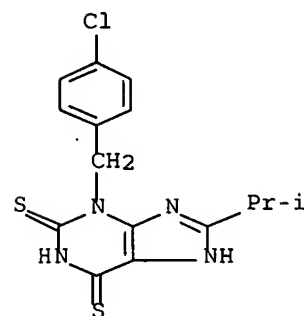
RN 162279-02-9 CAPLUS

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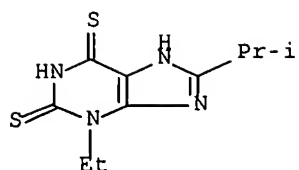
RN 162279-06-3 CAPLUS

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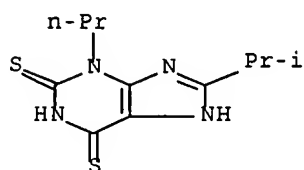
RN 162279-07-4 CAPLUS

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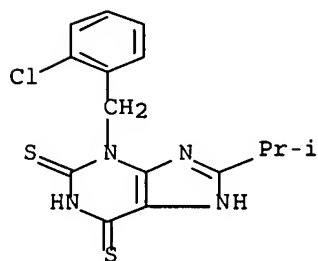
RN 162279-08-5 CAPLUS

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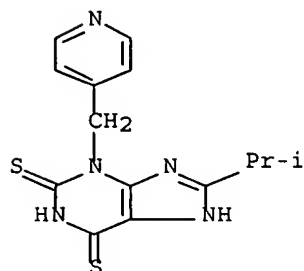
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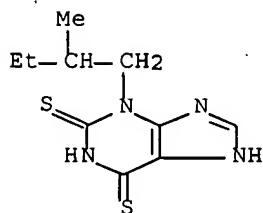
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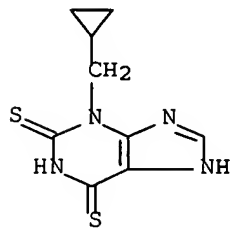
RN 300783-45-3 CAPLUS

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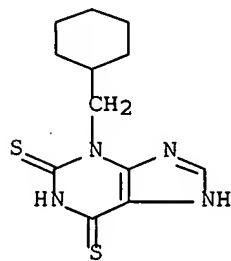
RN 300783-48-6 CAPLUS

CN 1H-Purine-2,6-dithione, 3-(cyclopropylmethyl)-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 300783-53-3 CAPLUS

CN 1H-Purine-2,6-dithione, 3-(cyclohexylmethyl)-3,7-dihydro- (9CI) (CA INDEX NAME)



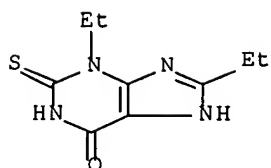
IT 162278-04-8, 3,8-Diethyl-2-thioxanthine

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of purine derivs. as phosphodiesterase IV inhibitors)

RN 162278-04-8 CAPLUS

CN 6H-Purin-6-one, 3,8-diethyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



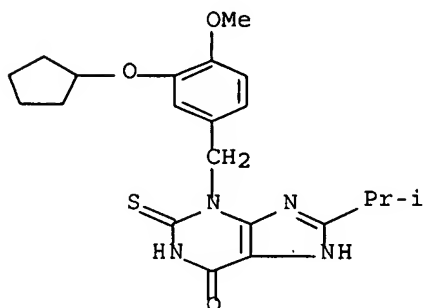
IT 300781-30-0P 300781-35-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of purine derivs. as phosphodiesterase IV inhibitors)

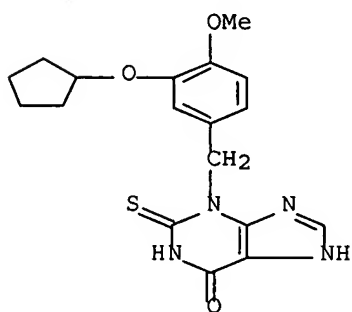
RN 300781-30-0 CAPLUS

CN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,2,3,7-tetrahydro-8-(1-methylethyl)-2-thioxo- (9CI) (CA INDEX NAME)



RN 300781-35-5 CAPLUS

CN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 10 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:721225 CAPLUS Full-text

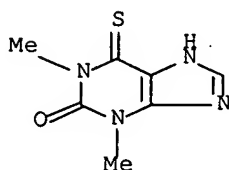
DOCUMENT NUMBER: 134:28992

TITLE: Solvent-free synthesis of thio-alkylxanthines from alkylxanthines using microwave irradiation

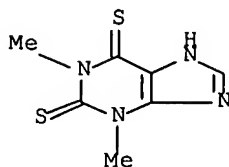
AUTHOR(S): Rico-Gomez, Rodrigo; Najera, Francisco; Lopez-Romero, Juan Manuel; Canada-Rudner, Pedro

CORPORATE SOURCE: Departamento de Quimica Organica. Universidad de

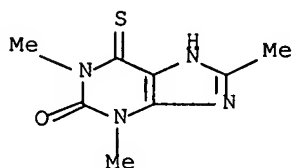
SOURCE: Malaga, E-29071, Spain  
 Heterocycles (2000), 53(10), 2275-2278  
 CODEN: HTCYAM; ISSN: 0385-5414  
 PUBLISHER: Japan Institute of Heterocyclic Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 134:28992  
 ED Entered STN: 13 Oct 2000  
 AB An expeditious, solvent-free procedure for the conversion of the xanthine bases theophylline, 8-methyltheophylline, caffeine, and theobromine to the corresponding 6-thio and 2,6-dithio derivs. using Lawesson's reagent under microwave irradiation is proposed.  
 IT 2398-70-1P, 6-Thiotheophylline 6501-94-6P  
 42459-09-6P 310904-66-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (solvent-free synthesis of thioalkylxanthines from alkylxanthines using microwave irradiation)  
 RN 2398-70-1 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 6501-94-6 CAPLUS  
 CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)

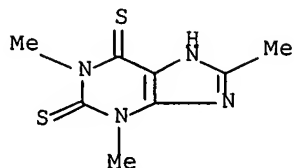


RN 42459-09-6 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3,8-trimethyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 310904-66-6 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3,8-trimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 11 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:544279 CAPLUS Full-text

DOCUMENT NUMBER: 133:281955

TITLE: New synthetic approach to theophylline and 6-thiotheophylline nucleosides from glycosyl derivatives of 4, 5-diaminouracil

AUTHOR(S): Rico-Gomez, Rodrigo; Lopez-Romero, Juan Manuel

CORPORATE SOURCE: Department de Quimica Organica, Facultad de Ciencias, Department de Quimica Organica, Facultad de Ciencias, Universidad de Malaga, Malaga, E-29071, Spain

SOURCE: Recent Research Developments in Organic & Bioorganic Chemistry (1999), 3, 93-106  
CODEN: RDOBFG

PUBLISHER: Transworld Research Network

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

ED Entered STN: 09 Aug 2000

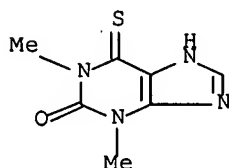
AB A review with 75 refs. on the syntheses of 7-theophylline nucleosides with special emphasis in the methods of construction of theophylline ring from 5-glycosylaminouracil. Preparation of 6-thiotheophylline nucleosides is also discussed.

IT 2398-70-1P, 6-Thiotheophylline

RL: SPN (Synthetic preparation); PREP (Preparation)  
(nucleoside derivs.; new synthetic approach to theophylline and thiotheophylline nucleosides from glycosyl derivs. of diaminouracil)

RN 2398-70-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)

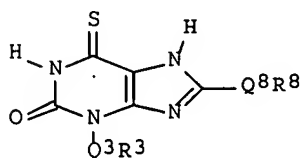


REFERENCE COUNT: 113 THERE ARE 113 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 12 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:344117 CAPLUS Full-text  
 DOCUMENT NUMBER: 132:347579  
 TITLE: Preparation of aryl thioxanthines as PDE IV inhibitors  
 INVENTOR(S): Cavalla, David; Hofer, Peter; Chasin, Mark  
 PATENT ASSIGNEE(S): Euro-Celtique S.A., Luxembourg  
 SOURCE: U.S., 12 pp., Cont.-in-part of U.S. Ser. No. 354,664,  
 abandoned.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 21  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6066641	A	20000523	US 1997-860680	19970611 <--
IN 180930	A1	19980404	IN 1995-CA1508	19951123 <--
IN 181538	A1	19980711	IN 1995-CA1506	19951123 <--
WO 9618399	A1	19960620	WO 1995-US16723	19951212 <--
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 6440979	B1	20020827	US 2000-547898	20000412 <--
PRIORITY APPLN. INFO.:			US 1994-354664	B2 19941213 <--
			WO 1995-US16723	W 19951212 <--
			IN 1994-CA514	A1 19940630 <--
			US 1997-860680	A1 19970611 <--
OTHER SOURCE(S): MARPAT 132:347579				
ED Entered STN: 24 May 2000				
GI				



AB The title compds. [I; Q3 = a bond, alkylene, alkenylene, alkynylene; Q8 =  
 alkylene, alkenylene, alkynylene; R3 = H, (un)substituted aryl, pyridyl, etc.;  
 R8 = H, (un)substituted aryl, pyrimidinyl, etc.; provided that Q3R3 is not H  
 or Me; and at least one of R3 and R8 = aryl, pyridyl, pyrimidinyl, quinolinyl  
 or isoquinolinyl] which possess PDE-IV inhibitory activity and improved  
 selectivity with regard to PDE-III inhibition, were prepared E.g., a multi-  
 step synthesis of I [Q3R3 = 3-cyclopentyloxy-4- methoxybenzyl; Q8R8 = iso-Pr]  
 which showed IC50 of 1.0  $\mu$ M against PDE IV vs. IC50 of 2.8  $\mu$ M against PDE IV  
 for rolipram in the same assay, was given.

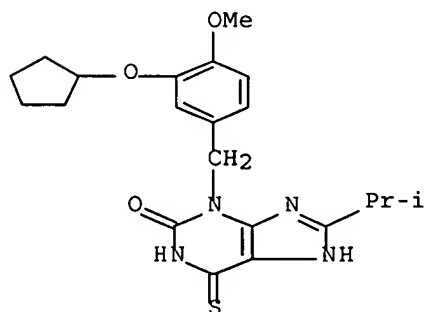
IT 179486-28-3P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological



study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of aryl thioxanthines as PDE IV inhibitors)

RN 179486-28-3 CAPLUS

CN 2H-Purin-2-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)

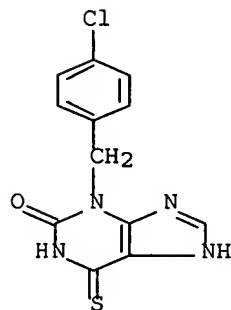


IT 179486-29-4P 179486-30-7P 179486-31-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of aryl thioxanthines as PDE IV inhibitors)

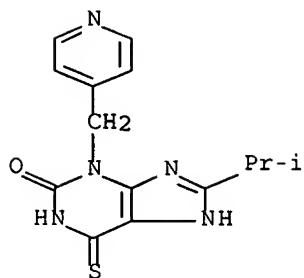
RN 179486-29-4 CAPLUS

CN 2H-Purin-2-one, 3-[(4-chlorophenyl)methyl]-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



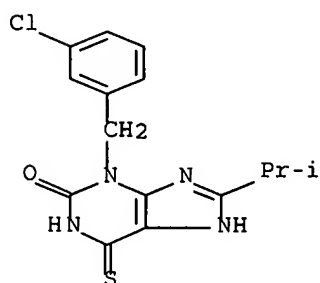
RN 179486-30-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-8-(1-methylethyl)-3-(4-pyridinylmethyl)-6-thioxo- (9CI) (CA INDEX NAME)



RN 179486-31-8 CAPLUS

CN 2H-Purin-2-one, 3-[(3-chlorophenyl)methyl]-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)

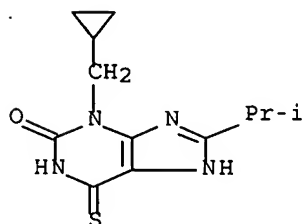


IT 179486-64-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of aryl thioxanthines as PDE IV inhibitors)

RN 179486-64-7 CAPLUS

CN 2H-Purin-2-one, 3-(cyclopropylmethyl)-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)

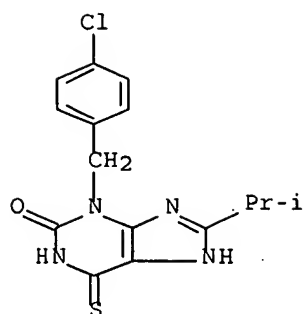


IT 179486-60-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of aryl thioxanthines as PDE IV inhibitors)

RN 179486-60-3 CAPLUS

CN 2H-Purin-2-one, 3-[(4-chlorophenyl)methyl]-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 178 THERE ARE 178 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

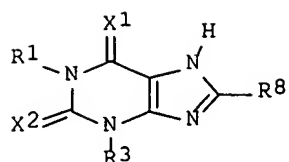
L57 ANSWER 13 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2000:113098 CAPLUS Full-text  
 DOCUMENT NUMBER: 132:151831  
 TITLE: Preparation of thioxanthines as PDE IV inhibitors  
 INVENTOR(S): Cavalla, David; Hofer, Peter; Chasin, Mark  
 PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg  
 SOURCE: U.S., 12 pp., Cont.-in-part of U.S. Ser. No. 476,262, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 21  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6025361	A	20000215	US 1997-860674	19970929 <--
IN 180930	A1	19980404	IN 1995-CA1508	19951123 <--
IN 181538	A1	19980711	IN 1995-CA1506	19951123 <--
CA 2206804	A1	19960620	CA 1995-2206804	19951212 <--
CA 2206804	C	20020319		
WO 9618400	A1	19960620	WO 1995-US16724	19951212 <--
W: AL, AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
IN 1995CA01665	A	20050304	IN 1995-CA1665	19951218 <--
US 5977119	A	19991102	US 1997-931849	19970915 <--
US 6268373	B1	20010731	US 1999-361196	19990726 <--
PRIORITY APPLN. INFO.:			US 1994-354664	B2 19941213 <--
			US 1995-476262	B2 19950607 <--
			WO 1995-US16724	W 19951212 <--
			IN 1994-CA514	A1 19940630 <--
			US 1997-860674	A1 19970929 <--

OTHER SOURCE(S): MARPAT 132:151831  
 ED Entered STN: 17 Feb 2000  
 GI



I

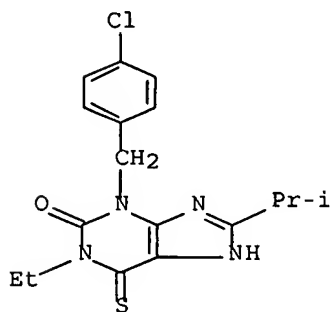
AB Title compds. [I; R1,R3,R8 = alkyl or aryl(alkyl); 1 of X1,X2 = S and the other = O or S] were prepared. Thus, 5,6-diamino-1,3-diethyl-2-thiouracil was N-acylated by cyclopropanecarbonyl chloride and the cyclized product treated with P4S10 to give I (R1 = R3 = Et, X1 = X2 = S). Data for biol. activity of I were given.

IT 179951-27-0P 179951-29-2P 179951-30-5P  
 179951-31-6P 179951-32-7P 179951-35-0P  
 179951-37-2P 179951-38-3P 179951-40-7P  
 179951-41-8P 257939-27-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of thioxanthines as PDE IV inhibitors)

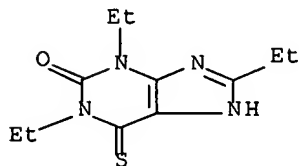
RN 179951-27-0 CAPLUS

CN 2H-Purin-2-one, 3-[(4-chlorophenyl)methyl]-1-ethyl-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



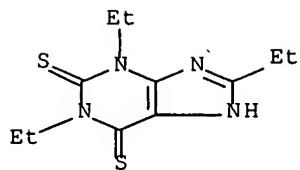
RN 179951-29-2 CAPLUS

CN 2H-Purin-2-one, 1,3,8-triethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



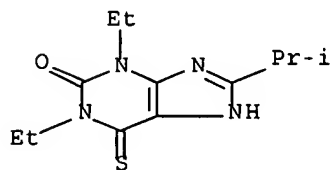
RN 179951-30-5 CAPLUS

CN 1H-Purine-2,6-dithione, 1,3,8-triethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



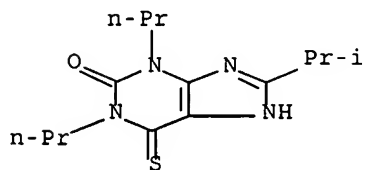
RN 179951-31-6 CAPLUS

CN 2H-Purin-2-one, 1,3-diethyl-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo-  
(9CI) (CA INDEX NAME)



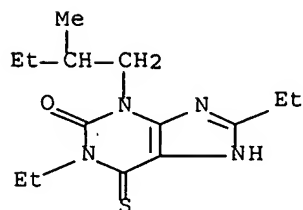
RN 179951-32-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-8-(1-methylethyl)-1,3-dipropyl-6-thioxo-  
(9CI) (CA INDEX NAME)



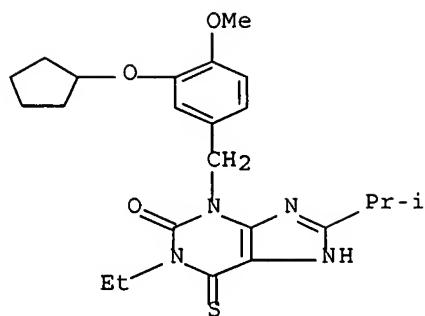
RN 179951-35-0 CAPLUS

CN 2H-Purin-2-one, 1,8-diethyl-1,3,6,7-tetrahydro-3-(2-methylbutyl)-6-thioxo-  
(9CI) (CA INDEX NAME)



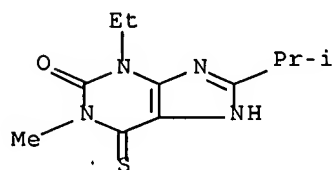
RN 179951-37-2 CAPLUS

CN 2H-Purin-2-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1-ethyl-  
1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



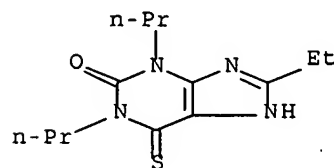
RN 179951-38-3 CAPLUS

CN 2H-Purin-2-one, 3-ethyl-1,3,6,7-tetrahydro-1-methyl-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



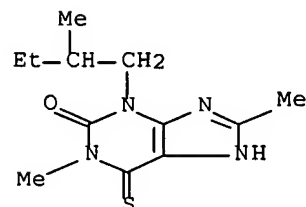
RN 179951-40-7 CAPLUS

CN 2H-Purin-2-one, 8-ethyl-1,3,6,7-tetrahydro-1,3-dipropyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 179951-41-8 CAPLUS

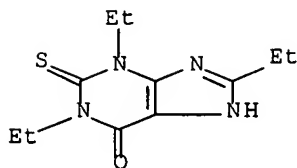
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,8-dimethyl-3-(2-methylbutyl)-6-thioxo- (9CI) (CA INDEX NAME)



RN 257939-27-8 CAPLUS

CN 6H-Purin-6-one, 1,3,8-triethyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA

INDEX NAME)



REFERENCE COUNT: 186 THERE ARE 186 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 14 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:34744 CAPLUS Full-text

DOCUMENT NUMBER: 132:88180

TITLE: Condensed purine derivatives as remedies for diabetes

INVENTOR(S): Shimada, Junichi; Ohta, Yoshihisa; Takasaki, Kotaro; Suda, Miho; Kusaka, Hideaki; Yano, Hiroshi; Nakanishi, Satoshi; Matsuda, Yuzuru

PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan

SOURCE: PCT Int. Appl., 98 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

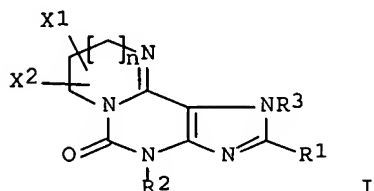
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000001388	A1	20000113	WO 1999-JP3583	19990702 <--
W: AU, BG, BR, CA, CN, CZ, HU, ID, IL, IN, JP, KR, MX, NO, NZ, PL, RO, SG, SI, SK, UA, US, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2336412	A1	20000113	CA 1999-2336412	19990702 <--
AU 9943968	A	20000124	AU 1999-43968	19990702 <--
EP 1092435	A1	20010418	EP 1999-926903	19990702 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
US 6489331	B1	20021203	US 2001-719570	20010409 <--
PRIORITY APPLN. INFO.:			JP 1998-187705	A 19980702 <--
			WO 1999-JP3583	W 19990702 <--

ED Entered STN: 14 Jan 2000

GI



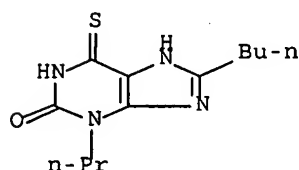
I

AB Remedies for diabetes which contain condensed purine derivs. as the active ingredient compds. represented by general formula (I) or physiol. acceptable salts thereof wherein R1 represents hydrogen, lower alkyl, optionally substituted aryl or optionally substituted heteroaryl; R2 represents hydrogen, lower alkyl, optionally substituted aralkyl, optionally substituted aryl or optionally substituted heteroaryl; R3 represents hydrogen, lower alkyl or optionally substituted aralkyl; X1 and X2 independently represent each hydrogen, lower alkyl, optionally substituted aralkyl or optionally substituted aryl; and n is an integer from 0 to 3. I can promote insulin secretion. Formulation examples of I were given.

IT 114834-11-6 254427-32-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensed purine derivs. as remedies for diabetes)

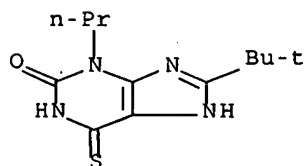
RN 114834-11-6 CAPLUS

CN 2H-Purin-2-one, 8-butyl-1,3,6,7-tetrahydro-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 254427-32-2 CAPLUS

CN 2H-Purin-2-one, 8-(1,1-dimethylethyl)-1,3,6,7-tetrahydro-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 15 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:491591 CAPLUS Full-text

DOCUMENT NUMBER: 131:257779

TITLE: 15N-Multi-labeled Adenine and Guanine Nucleosides. Syntheses of [1,3,NH2-15N3]- and [2-13C-1,3,NH2-15N3]-Labeled Adenosine, Guanosine, 2'-Deoxyadenosine, and 2'-Deoxyguanosine

AUTHOR(S): Abad, Jose-Luis; Gaffney, Barbara L.; Jones, Roger A.

CORPORATE SOURCE: Department of Chemistry, Rutgers The State University of New Jersey, Piscataway, NJ, 08854, USA

SOURCE: Journal of Organic Chemistry (1999), 64(18), 6575-6582

CODEN: JOCEAH; ISSN: 0022-3263



PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

ED Entered STN: 10 Aug 1999

AB The authors report a high-yield route to the following specifically  $^{15}\text{N}$ - and  $^{13}\text{C}$ -multi-labeled nucleosides:  $[1,3,\text{NH}_2\text{-}^{15}\text{N}_3]\text{-}$  and  $[2\text{-}^{13}\text{C}\text{-}1,3,\text{NH}_2\text{-}^{15}\text{N}_3]\text{-}$  adenosine;  $[1,3,\text{NH}_2\text{-}^{15}\text{N}_3]\text{-}$  and  $[2\text{-}^{13}\text{C}\text{-}1,3,\text{NH}_2\text{-}^{15}\text{N}_3]\text{-}$  guanosine;  $[1,3,\text{NH}_2\text{-}^{15}\text{N}_3]\text{-}$  and  $[2\text{-}^{13}\text{C}\text{-}1,3,\text{NH}_2\text{-}^{15}\text{N}_3]\text{-}2'\text{-deoxyadenosine}$ ;  $[1,3,\text{NH}_2\text{-}^{15}\text{N}_3]\text{-}$  and  $[2\text{-}^{13}\text{C}\text{-}1,3,\text{NH}_2\text{-}^{15}\text{N}_3]\text{-}2'\text{-deoxyguanosine}$ . In each set, the  $^{13}\text{C}_2$  atom functions as a "tag" that allows the  $^{15}\text{N}_1$  and  $^{15}\text{N}_3$  atoms to be unambiguously differentiated from the untagged versions in  $^{15}\text{N}$  NMR of RNA or DNA fragments. The key intermediate of this synthetic strategy for both the adenine and guanine nucleosides is  $[\text{NH}_2,\text{CONH}_2\text{-}^{15}\text{N}_2]\text{-}5\text{-amino-}4\text{-imidazolecarboxamide}$ . The  $[2\text{-}^{13}\text{C}]\text{-}$  label is added through a ring closure using  $[^{13}\text{C}]\text{-sodium Et xanthate}$  ( $\text{NaS}^{13}\text{CSOEt}$ ). Enzymic transglycosylation of either multi-labeled 6-chloropurine or multi-labeled 2-mercaptopyoxanthine and a final reaction with  $^{15}\text{NH}_3$  give the adenine and guanine nucleosides. This is the first report of a  $[3\text{-}^{15}\text{N}]\text{-}$ labeled guanine nucleoside.

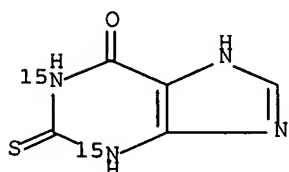
IT 244769-62-8P 244769-79-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(syntheses of  $[^{15}\text{N}_3]\text{-}$  and  $[^{13}\text{C},^{15}\text{N}_3]\text{-}$ labeled adenosine, guanosine, deoxyadenosine, and deoxyguanosine nucleosides)

RN 244769-62-8 CAPLUS

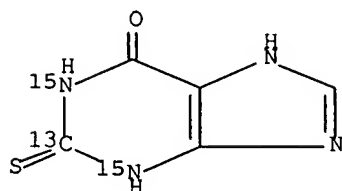
CN 6H-Purin-6-one-1,3- $^{15}\text{N}_2$ , 1,2,3,7-tetrahydro-2-thioxo-, monosodium salt (9CI) (CA INDEX NAME)



● Na

RN 244769-79-7 CAPLUS

CN 6H-Purin-6-one-2- $^{13}\text{C}\text{-}1,3\text{-}^{15}\text{N}_2$ , 1,2,3,7-tetrahydro-2-thioxo-, monosodium salt (9CI) (CA INDEX NAME)



● Na

REFERENCE COUNT: 7

21

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 16 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:412389 CAPLUS Full-text

DOCUMENT NUMBER: 131:179928

TITLE: 1,3-Dialkylxanthine derivatives having high potency as antagonists at human A2b adenosine receptors

AUTHOR(S): Jacobson, Kenneth A.; Ijzerman, Ad P.; Linden, Joel

CORPORATE SOURCE: Molecular Recognition Section, Laboratory of Bioorganic Chemistry, National Institute of Diabetes, Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD, 20892-0810, USA

SOURCE: Drug Development Research (1999), 47(1), 45-53

CODEN: DDREDK; ISSN: 0272-4391

PUBLISHER: Wiley-Liss, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 05 Jul 1999

AB The structure-activity relationships (SAR) of alkylxanthine derivs. as antagonists at the recombinant human adenosine receptors were explored in order to identify selective antagonists of A2B receptors. The effects of lengthening alkyl substituents from Me to Bu at 1- and 3-positions and addnl. substitution at the 7- and 8-positions were probed. Ki values, determined in competition binding in membranes of HEK-293 cells expressing A2B receptors using 125I-ABOPX (125I-3-(4-amino-3-iodobenzyl)-8-(phenyl-4- oxyacetate)-1-propylxanthine), were approx. 10 to 100 nM for 8-phenylxanthine functionalized congeners. Xanthines containing 8-aryl, 8-alkyl, and 8-cycloalkyl substituents, derivs. of XCC (8-[4-[[[carboxy]methyl]oxy]phenyl]-1,3-dipropylxanthine) and XAC (8-[4-[[[(2-amino-ethyl)amino]carbonyl]methyl]oxy]phenyl]-1,3- dipropylxanthine), containing various ester and amide groups, including L- and D-amino acid conjugates, were included. Enprofylline was 2-fold more potent than theophylline in A2B receptor binding, and the 2-thio modification was not tolerated. Among the most potent derivs. examined were XCC, its hydrazide and aminoethyl and fluoroethyl amide derivs., XAC, N-hydroxyethyl-XAC, and the L-citrulline and D-p-aminophenylalanine conjugates of XAC. An N-hydroxysuccinimide ester of XCC (XCC-NHS, MRS 1204) bound to A2B receptors with a Ki of 9.75 nM and was the most selective (at least 20-fold) in this series. In a functional assay of recombinant human A2B receptors, four of these potent xanthines were shown to fully antagonize the effects of NECA-induced stimulation of cAMP accumulation.

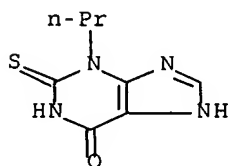
IT 156733-29-8

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(1,3-Dialkylxanthine derivs. having high potency as antagonists at human A2b adenosine receptors)

RN 156733-29-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-propyl-2-thioxo- (9CI) (CA INDEX NAME)

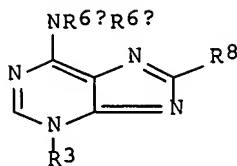


REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

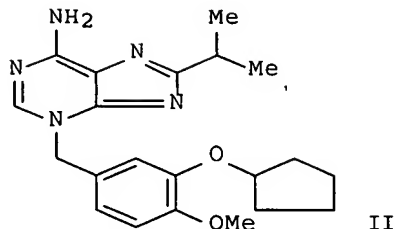
L57 ANSWER 17 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1999:404966 CAPLUS Full-text  
 DOCUMENT NUMBER: 131:58700  
 TITLE: Preparation of purine derivatives having  
 phosphodiesterase IV inhibiting activity  
 INVENTOR(S): Cavalla, David; Chasin, Mark; Hofer, Peter; Gehrig,  
 Andre; Wintergerst, Peter  
 PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg  
 SOURCE: PCT Int. Appl., 44 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 21  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9931102	A1	19990624	WO 1998-US26293	19981211 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
IN 180930	A1	19980404	IN 1995-CA1508	19951123 <--
IN 181538	A1	19980711	IN 1995-CA1506	19951123 <--
US 6037470	A	20000314	US 1998-209658	19981210 <--
US 6040447	A	20000321	US 1998-209922	19981210 <--
US 6057445	A	20000502	US 1998-209664	19981210 <--
CA 2314335	A1	19990624	CA 1998-2314335	19981211 <--
AU 9918159	A	19990705	AU 1999-18159	19981211 <--
AU 747366	B2	20020516		
BR 9815171	A	20001010	BR 1998-15171	19981211 <--
EP 1045849	A1	20001025	EP 1998-963053	19981211 <--
EP 1045849	B1	20030702		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
TR 200001706	T2	20001121	TR 2000-200001706	19981211 <--
US 6211367	B1	20010403	US 1998-210557	19981211 <--
US 6228859	B1	20010508	US 1998-210556	19981211 <--
HU 200100417	A2	20011228	HU 2001-417	19981211 <--
JP 2002508376	T	20020319	JP 2000-539025	19981211 <--
JP 3504234	B2	20040308		
AT 244243	T	20030715	AT 1998-963053	19981211 <--
PT 1045849	T	20031128	PT 1998-963053	19981211 <--
ES 2202924	T3	20040401	ES 1998-963053	19981211 <--
NO 2000002998	A	20000719	NO 2000-2998	20000609 <--
PRIORITY APPLN. INFO.:			US 1997-69371P	P 19971212 <--
			IN 1994-CA514	A1 19940630 <--
			WO 1998-US26293	W 19981211 <--

OTHER SOURCE(S): MARPAT 131:58700  
 ED Entered STN: 01 Jul 1999  
 GI



I



II

AB Purines I [R3 = alkyl, alkenyl, cycloalkyl, cycloalkenyl, wherein said alkyl, alkenyl, cycloalkyl, cycloalkylalkyl, cycloalkenyl; R6a, R6b = H, alkyl, alkenyl, cycloalkyl, cycloalkenyl; R8 = H, alkyl, alkenyl, cycloalkyl, cycloalkenyl] were prepared for use as phosphodiesterase inhibitors for the treatment of diseases such as asthma, allergy, or inflammation. Thus, purine derivative II was prepared starting from 3-(3-cyclopentyloxy-4-methoxybenzyl)-8-isopropylhypoxanthine. The prepared purines were tested for inhibitory activity against phosphodiesterase types III, IV, and V.

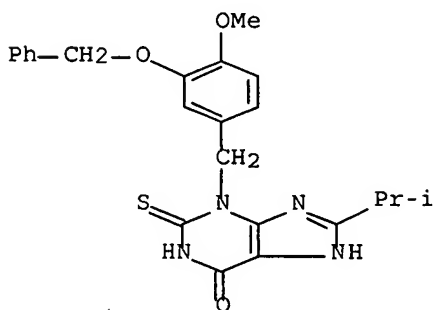
IT 227763-83-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of purine derivs. having phosphodiesterase IV inhibition activity)

RN 227763-83-9 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-[[4-methoxy-3-(phenylmethoxy)phenyl]methyl]-8-(1-methylethyl)-2-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 18 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:441960 CAPLUS Full-text

DOCUMENT NUMBER: 129:109311

TITLE: Preparation of nucleoside uronamides as A3 adenosine receptor agonists

INVENTOR(S): Jacobson, Kenneth A.; Gallo-Rodriguez, Carola; Van Galen, Philip J. M.; Von Lubitz, Dag K. J. E.; Jeong, Heaok Kim

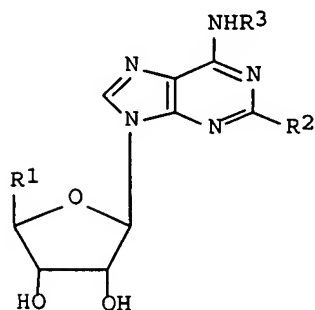
PATENT ASSIGNEE(S): United States Dept. of Health and Human Services, USA

SOURCE: U.S., 54 pp., Cont.-in-part of U. S. Ser. No. 163,324, abandoned.

CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5773423	A	19980630	US 1994-274628	19940713 <--
US 5688774	A	19971118	US 1995-396111	19950228 <--
PRIORITY APPLN. INFO.:			US 1993-91109	B2 19930713 <--
			US 1993-163324	B2 19931206 <--
			US 1994-274628	A2 19940713 <--

OTHER SOURCE(S): MARPAT 129:109311  
 ED Entered STN: 17 Jul 1998  
 GI



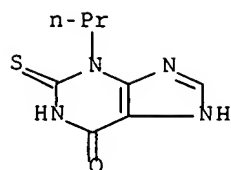
AB The present invention provides N6-benzyladenosine-5'-N-uronamide and related substituted compds. I (R1 = amide; R2 = halo, amino, alkenyl, alkynyl, thio, alkylthio; R3 = S-1-phenylethyl, Bn, phenylethyl), particularly those containing substituents on the benzyl and/or uronamide groups, and modified xanthine ribosides, as well as pharmaceutical compns. containing such compds. The present invention also provides a method of selectively activating an A3 adenosine receptor in a mammal, which method comprises acutely or chronically administering to a mammal in need of selective activation of its A3 adenosine receptor a therapeutically effective amount of a compound which binds with the A3 receptor so as to stimulate an A3 receptor-dependent response. Thus, N6-(3-iodobenzyl)adenosine was prepared tested for its affinity in binding at rat brain A1, A2, A3 adenosine receptors (Ki = 9.5-220.0 nM).

IT 156733-29-8P

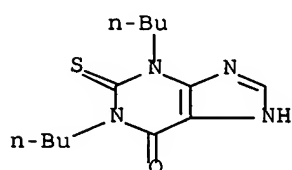
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of nucleoside uronamides as A3 adenosine receptor agonists)

RN 156733-29-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-propyl-2-thioxo- (9CI) (CA INDEX NAME)



IT 77038-96-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of nucleoside uronamides as A3 adenosine receptor agonists)  
 RN 77038-96-1 CAPLUS  
 CN 6H-Purin-6-one, 1,3-dibutyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 19 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1998:153640 CAPLUS Full-text  
 DOCUMENT NUMBER: 128:303616  
 TITLE: Correlations of PDE-4 inhibition between enzymes of smooth muscle and inflammatory cell sources  
 AUTHOR(S): Cariuk, Peter; Cavalla, David; Chasin, Mark; Giembycz, Mark  
 CORPORATE SOURCE: Napp Research Centre, Cambridge Science Park, Cambridge, CB4 4GW, UK  
 SOURCE: Cell Biochemistry and Biophysics (1998), 28(2-3), 219-249  
 CODEN: CBBIFV; ISSN: 1085-9195  
 PUBLISHER: Humana Press Inc.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 14 Mar 1998  
 AB The sensitivities of PDE-4 enzymes from smooth muscle and inflammatory cell sources from different species to a range of structurally diverse compds. were compared. All inflammatory cell PDE-4 sources displayed good cross-correlations in their sensitivity to inhibition by these compds. Similarly, PDE-4 enzymes from smooth muscle sources were well-correlated; however, there was no cross-correlation between PDE-4 from smooth muscle sources and those of inflammatory cell sources, possibly reflecting differences in subcellular location of enzymes as well as subtype expression. The present study concludes that PDE-4 prepns. from smooth muscle sources as well as those from inflammatory cell sources can be used to model the potential smooth muscle cell relaxing properties and antiinflammatory properties of a compound in relation to human asthma.  
 IT 162279-04-1 179486-28-3 179486-64-7  
 179951-31-6 179951-32-7 179951-37-2

179951-38-3 206352-05-8 206352-07-0

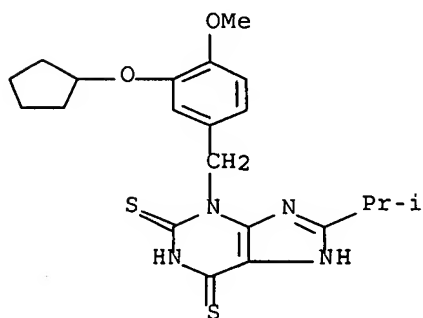
206352-09-2 206352-16-1

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(correlations of PDE-4 inhibition between enzymes of smooth muscle and inflammatory cell sources)

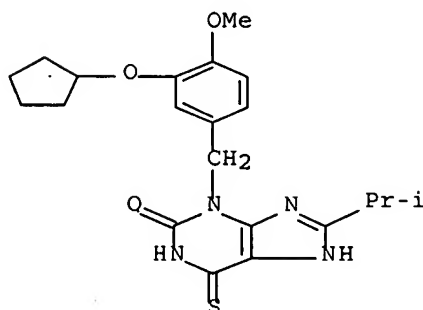
RN 162279-04-1 CAPLUS

CN 1H-Purine-2,6-dithione, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



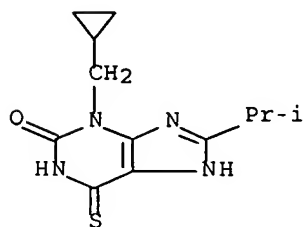
RN 179486-28-3 CAPLUS

CN 2H-Purin-2-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)

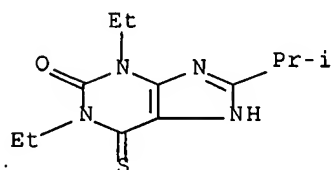


RN 179486-64-7 CAPLUS

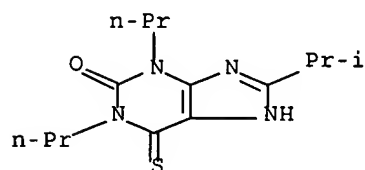
CN 2H-Purin-2-one, 3-(cyclopropylmethyl)-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



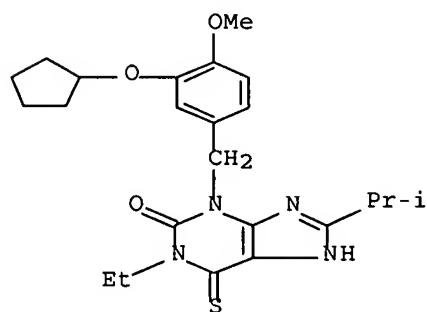
RN 179951-31-6 CAPLUS

CN 2H-Purin-2-one, 1,3-diethyl-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo-  
(9CI) (CA INDEX NAME)

RN 179951-32-7 CAPLUS

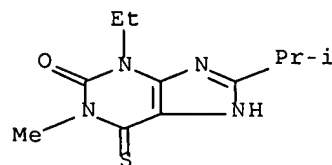
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-8-(1-methylethyl)-1,3-dipropyl-6-thioxo-  
(9CI) (CA INDEX NAME)

RN 179951-37-2 CAPLUS

CN 2H-Purin-2-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1-ethyl-  
1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)

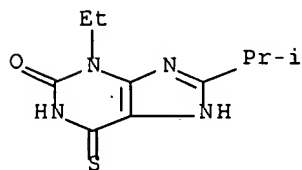
RN 179951-38-3 CAPLUS

CN 2H-Purin-2-one, 3-ethyl-1,3,6,7-tetrahydro-1-methyl-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)

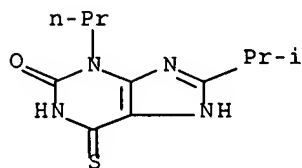




RN 206352-05-8 CAPLUS

CN 2H-Purin-2-one, 3-ethyl-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo-  
(9CI) (CA INDEX NAME)

RN 206352-07-0 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-8-(1-methylethyl)-3-propyl-6-thioxo-  
(9CI) (CA INDEX NAME)

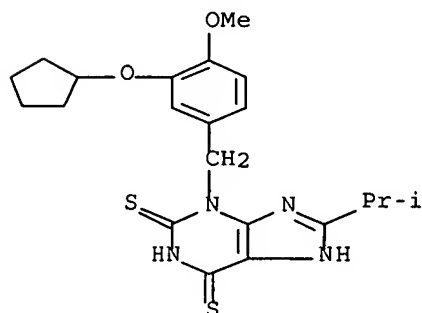
RN 206352-09-2 CAPLUS

CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-(1-methylethyl)-1H-purine-2,6-dithione (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 162279-04-1

CMF C21 H26 N4 O2 S2



CM 2

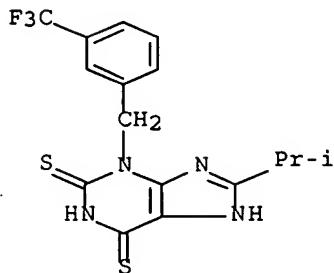
CRN 62-49-7

CMF C5 H14 N O

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RN 206352-16-1 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-[[3-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 20 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:331961 CAPLUS Full-text

DOCUMENT NUMBER: 126:305588

TITLE: Preparation of 4-(dioxopurinylmethyl)phenylacetates and analogs as hypolipemics

INVENTOR(S): Connell, Richard; Goldmann, Siegfried; Mueller, Ulrich; Lohmer, Stefan; Bischoff, Hilmar; Denzer, Dirk; Gruetzmann, Rudi; Wohlfeil, Stefan

PATENT ASSIGNEE(S): Bayer A.-G., Germany

SOURCE: Eur. Pat. Appl., 69 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

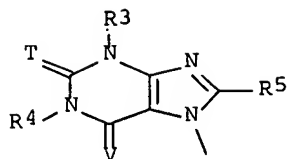
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 764647	A1	19970326	EP 1996-114577	19960912 <--
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
DE 19535504	A1	19970327	DE 1995-19535504	19950925 <--
US 5714494	A	19980203	US 1996-710503	19960918 <--
JP 09216884	A	19970819	JP 1996-267691	19960919 <--
CA 2186086	A1	19970326	CA 1996-2186086	19960920 <--

PRIORITY APPLN. INFO.: DE 1995-19535504 A 19950925 &lt;--

OTHER SOURCE(S): MARPAT 126:305588

ED Entered STN: 24 May 1997

GI



II

AB RCH<sub>2</sub>ZCHR<sub>1</sub>C(:L)R<sub>2</sub> [I; R = xanthine moiety, e.g., II; R<sub>1</sub> = H, (cyclo)alkyl, Ph, heterocyclyl, etc.; R<sub>2</sub> = OH, SH, alkoxy, (di)alkylamino, etc.; R<sub>3</sub>, R<sub>4</sub> = H, alkyl, aryl, etc.; R<sub>5</sub> = H, halo, alkyl, aryl, etc.; L, T, V = O or S; Z = (un)substituted 1,4-phenylene] were prepared. Thus, 5,6-diamino-1,3-dimethyluracil was cyclocondensed with 4-MeC<sub>6</sub>H<sub>4</sub>CHO and the product N-alkylated by 4-(BrCH<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>CHR<sub>1</sub>CO<sub>2</sub>CMe<sub>3</sub> (R<sub>1</sub> = cyclopentyl) (preparation given) to give 4-(RCH<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>CHR<sub>1</sub>CO<sub>2</sub>CMe<sub>3</sub> (R = II, R<sub>1</sub> = cyclopentyl, R<sub>3</sub> = R<sub>4</sub> = Me, R<sub>5</sub> = C<sub>6</sub>H<sub>4</sub>Me-4, T = V = O). Data for biol. activity of I were given.

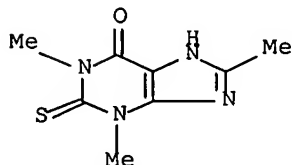
IT 19673-55-3P 189215-37-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 4-(dioxopurinylmethyl)phenylacetates and analogs as hypolipemics)

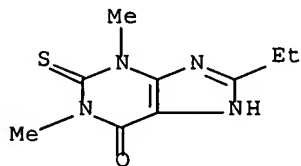
RN 19673-55-3 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3,8-trimethyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 189215-37-0 CAPLUS

CN 6H-Purin-6-one, 8-ethyl-1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 21 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:497159 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 125:142465

TITLE: Preparation of 1,3,8-trialkylthioxoxanthines as phosphodiesterase inhibitors

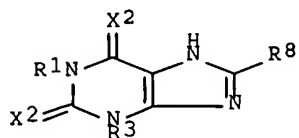
INVENTOR(S): Cavalla, David J.; Hofer, Peter; Chasin, Mark

PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg

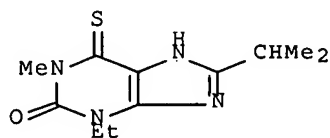
SOURCE: PCT Int. Appl., 37 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 21  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9618400	A1	19960620	WO 1995-US16724	19951212 <--
W: AL, AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
IN 180930	A1	19980404	IN 1995-CA1508	19951123 <--
IN 181538	A1	19980711	IN 1995-CA1506	19951123 <--
AU 9645279	A	19960703	AU 1996-45279	19951212 <--
EP 799040	A1	19971008	EP 1995-943950	19951212 <--
EP 799040	B1	20030820		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
JP 2001523213	T	20011120	JP 1996-519327	19951212 <--
AT 247655	T	20030915	AT 1995-943950	19951212 <--
US 6025361	A	20000215	US 1997-860674	19970929 <--
US 6268373	B1	20010731	US 1999-361196	19990726 <--
PRIORITY APPLN. INFO.:			US 1995-476262	A 19950607 <--
			IN 1994-CA514	A1 19940630 <--
			US 1994-354664	A 19941213 <--
			WO 1995-US16724	W 19951212 <--
			US 1997-860674	A1 19970929 <--

OTHER SOURCE(S): MARPAT 125:142465  
 ED Entered STN: 21 Aug 1996  
 GI



I



II

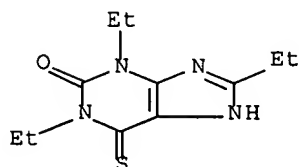
AB Title compds. [I; R1,R3,R8 = (ar)alkyl, aryl; 1 of X1,X2 = S and the other = O or S] were prepared. Thus, title compound II had IC50 of 1.0µM against phosphodiesterase IV and V in vitro.

IT 179951-29-2P 179951-30-5P 179951-31-6P  
 179951-32-7P 179951-35-0P 179951-37-2P  
 179951-38-3P 179951-40-7P 179951-41-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of 1,3,8-trialkylthioxoxanthines as phosphodiesterase inhibitors)

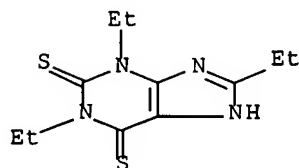
RN 179951-29-2 CAPLUS

CN 2H-Purin-2-one, 1,3,8-triethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



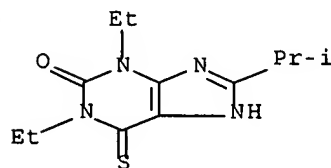
RN 179951-30-5 CAPLUS

CN 1H-Purine-2,6-dithione, 1,3,8-triethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



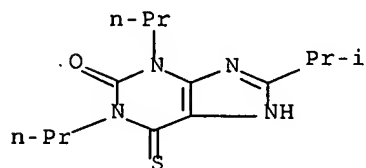
RN 179951-31-6 CAPLUS

CN 2H-Purin-2-one, 1,3-diethyl-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



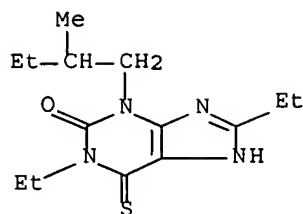
RN 179951-32-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-8-(1-methylethyl)-1,3-dipropyl-6-thioxo- (9CI) (CA INDEX NAME)



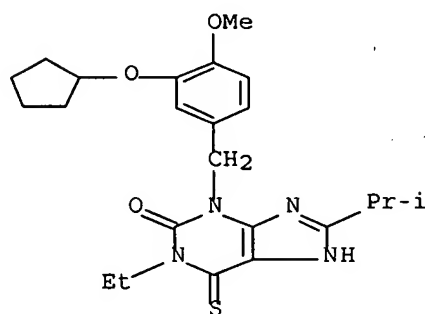
RN 179951-35-0 CAPLUS

CN 2H-Purin-2-one, 1,8-diethyl-1,3,6,7-tetrahydro-3-(2-methylbutyl)-6-thioxo- (9CI) (CA INDEX NAME)



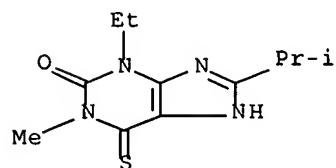
RN 179951-37-2 CAPLUS

CN 2H-Purin-2-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1-ethyl-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



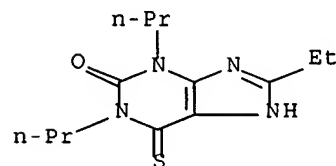
RN 179951-38-3 CAPLUS

CN 2H-Purin-2-one, 3-ethyl-1,3,6,7-tetrahydro-1-methyl-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)

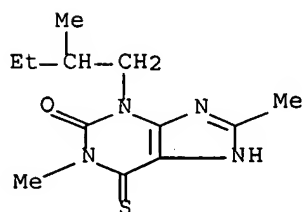


RN 179951-40-7 CAPLUS

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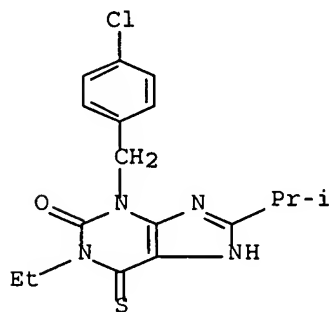
RN 179951-41-8 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,8-dimethyl-3-(2-methylbutyl)-6-thioxo-  
(9CI) (CA INDEX NAME)

IT 179951-27-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)(preparation of 1,3,8-trialkylthioxoxanthines as phosphodiesterase  
inhibitors)

RN 179951-27-0 CAPLUS

CN 2H-Purin-2-one, 3-[(4-chlorophenyl)methyl]-1-ethyl-1,3,6,7-tetrahydro-8-(1-  
methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)

L57 ANSWER 22 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:473245 CAPLUS Full-text

DOCUMENT NUMBER: 125:142764

TITLE: Preparation of aryl thioxanthines as phosphodiesterase  
inhibitors

INVENTOR(S): Cavalla, David J.; Hofer, Peter; Chasin, Mark

PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg

SOURCE: PCT Int. Appl., 40 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 21

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9618399	A1	19960620	WO 1995-US16723	19951212 <--
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ,				

TM, TT

RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE,  
IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR,  
NE, SN, TD, TG

IN 180930	A1	19980404	IN 1995-CA1508	19951123 <--
IN 181538	A1	19980711	IN 1995-CA1506	19951123 <--
CA 2206287	A1	19960620	CA 1995-2206287	19951212 <--
CA 2206287	C	20010320		
AU 9645278	A	19960703	AU 1996-45278	19951212 <--
EP 814809	A1	19980107	EP 1995-943949	19951212 <--
EP 814809	B1	20030813		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE

JP 10508032	T	19980804	JP 1995-519326	19951212 <--
AT 247116	T	20030815	AT 1995-943949	19951212 <--
ZA 9510594	A	19960619	ZA 1995-10594	19951213 <--
ZA 9510595	A	19960619	ZA 1995-10595	19951213 <--
IN 1995CA01664	A	20050304	IN 1995-CA1664	19951218 <--
US 6066641	A	20000523	US 1997-860680	19970611 <--
US 6090816	A	20000718	US 1997-911549	19970814 <--
US 6440979	B1	20020827	US 2000-547898	20000412 <--

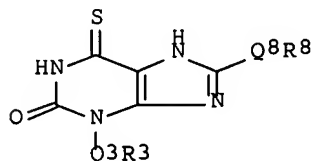
PRIORITY APPLN. INFO.:

US 1994-354664	A	19941213 <--
IN 1994-CA514	A1	19940630 <--
WO 1995-US16723	W	19951212 <--
US 1997-860680	A1	19970611 <--

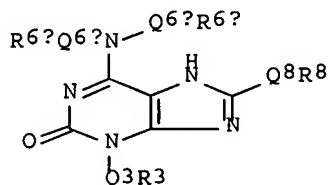
OTHER SOURCE(S): MARPAT 125:142764

ED Entered STN: 10 Aug 1996

GI



I



II

AB Title compds. I or II (Q3, Q6a, Q6b, Q8 are independently a bond, C1-8 alkylene, C2-8 alkenylene, C2-8 alkynylene; R3, R6a, R6b and R8 are independently H, aryl, heteroaryl, optionally substituted by halogen, hydroxy, alkoxy, nitro, cyano and carboxy, provided that Q3R3 is not H or Me in I or II, and at least one of R3 and R8 is aryl or heteroaryl in I), useful as phosphodiesterase inhibitors, are claimed. The compds. are effective PDE IV inhibitors and possess improved PDE IV inhibition and improved selectivity with regard to PDE III inhibition. Thus, the IC<sub>50</sub> for 3-(3-cyclopentyloxy-4-methoxybenzyl)-8-isopropyl-6-thioxanthine (preparation given) was 1.0 μM for PDE IV inhibition, compared with 2.8 μM for rolipram.

IT 179486-28-3P 179486-29-4P 179486-30-7P  
179486-31-8P

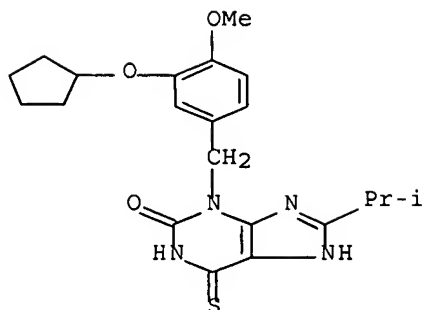
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aryl thioxanthines as phosphodiesterase inhibitors)

RN 179486-28-3 CAPLUS

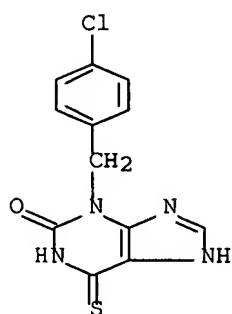
CN 2H-Purin-2-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)





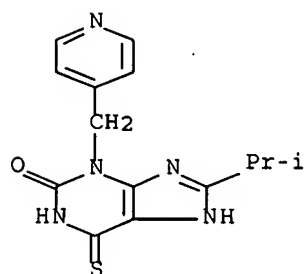
RN 179486-29-4 CAPLUS

CN 2H-Purin-2-one, 3-[(4-chlorophenyl)methyl]-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



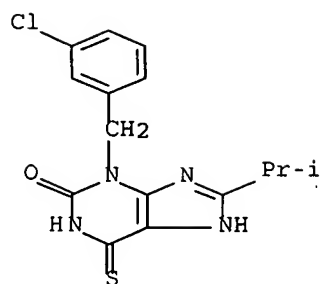
RN 179486-30-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-8-(1-methylethyl)-3-(4-pyridinylmethyl)-6-thioxo- (9CI) (CA INDEX NAME)



RN 179486-31-8 CAPLUS

CN 2H-Purin-2-one, 3-[(3-chlorophenyl)methyl]-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



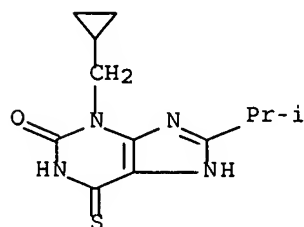
IT 179486-64-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of aryl thioxanthines as phosphodiesterase inhibitors)

RN 179486-64-7 CAPLUS

CN 2H-Purin-2-one, 3-(cyclopropylmethyl)-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



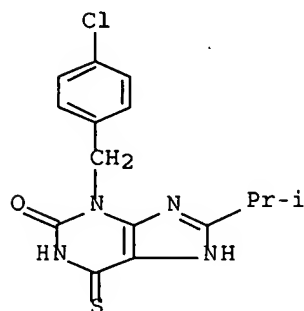
IT 179486-60-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of aryl thioxanthines as phosphodiesterase inhibitors)

RN 179486-60-3 CAPLUS

CN 2H-Purin-2-one, 3-[(4-chlorophenyl)methyl]-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



IT 179486-67-0

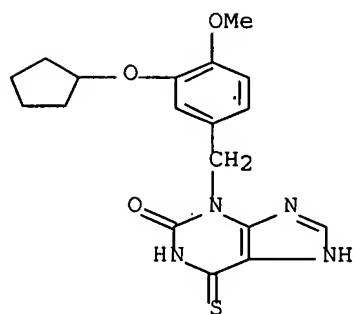
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of aryl thioxanthines as phosphodiesterase inhibitors)

RN 179486-67-0 CAPLUS

CN 2H-Purin-2-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,3,6,7-

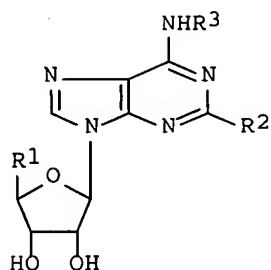
tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 23 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1995:837438 CAPLUS Full-text  
 DOCUMENT NUMBER: 123:257265  
 TITLE: Preparation of N6-benzyladenosine-5'-uronamides,  
 modified xanthine ribosides, and related compounds as  
 adenosine A3 receptor agonists.  
 INVENTOR(S): Jacobson, Kenneth A.; Gallo-Rodriguez, Carola; Von  
 Galen, Philip J. M.; Von Lubitz, Dag K. J. E.; Jeong,  
 Heaok Kim  
 PATENT ASSIGNEE(S): United States Dept. of Health and Human Services, USA  
 SOURCE: PCT Int. Appl., 175 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9502604	A1	19950126	WO 1994-US7835	19940713 <--
W: AU, CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9473310	A	19950213	AU 1994-73310	19940713 <--
EP 708781	A1	19960501	EP 1994-923445	19940713 <--
EP 708781	B1	20011004		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
AT 206432	T	20011015	AT 1994-923445	19940713 <--
PRIORITY APPLN. INFO.:				
			US 1993-91109	A 19930713 <--
			US 1993-163324	A 19931206 <--
			WO 1994-US7835	W 19940713 <--

OTHER SOURCE(S): MARPAT 123:257265  
 ED Entered STN: 07 Oct 1995  
 GI



I

AB Title compds. [I; R1 = RaRbNCO, HORc; Ra, Rb = H, alkyl, amino, haloalkyl, aminoalkyl, cycloalkyl, BOC-aminoalkyl; RaRbN = heterocyclyl; Rc = alkyl, amino, haloalkyl, aminoalkyl, cycloalkyl, BOC-aminoalkyl; R2 = H, halo, alkyl ether residue, amino, alkylamino, alkenyl, alkynyl, thio, alkylthio; R3 = (R)- and (S)-1-phenylethyl, (substituted) PhCH2, substituted phenylethyl] and related compds., were prepared Thus, 2-chloro-N6-(3-iodobenzyl)adenine was refluxed with hexamethyldisilazane and cat. (NH4)2SO4 to give a silyl derivative which was refluxed with N-Me I-O-acetyl-2,3-dibenzoyl- $\alpha,\beta$ -D-ribofuronamide and trimethylsilyl triflate in dichloroethane to give 2-chloro-N6-(3-iodobenzyl)-9-[5-(methyamido)-2,3-di-O-benzoyl- $\beta$ -D-ribofuranosyl]adenine. The latter was stirred with NH3 in MeOH for 16 h to give 68.7% 2-chloro-N6-(3-iodobenzyl)-9-[5-(methyamido)- $\beta$ -D-ribofuranosyl]adenine. This showed Ki = 0.23 nM in a radioligand binding assay at rat brain A3 receptors.

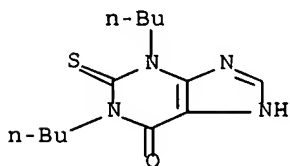
IT 77038-96-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of N6-benzyladenosine-5'-uronamides, modified xanthine ribosides, and related compds. as adenosine A3 receptor agonists)

RN 77038-96-1 CAPLUS

CN 6H-Purin-6-one, 1,3-dibutyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 24 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:492020 CAPLUS Full-text

DOCUMENT NUMBER: 122:239459

TITLE: Preparation of purines, isoguanines, and dithioxanthines as phosphodiesterase-IV inhibitors  
INVENTOR(S): Cavalla, David; Hofer, Peter; Gehrig, Anddre; Wintergest, Peter

PATENT ASSIGNEE(S): Euro-Celtique S.A., Luxembourg

SOURCE: PCT Int. Appl., 75 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 21

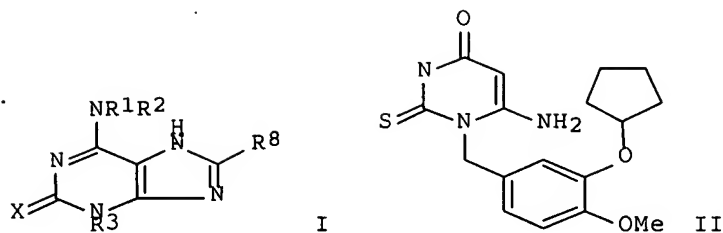
## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9500516	A1	19950105	WO 1994-GB1334	19940621 <--
W: AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2165433	A1	19941223	CA 1994-2165433	19940621 <--
CA 2165433	C	20020528		
AU 9469771	A	19950117	AU 1994-69771	19940621 <--
AU 683270	B2	19971106		
EP 705265	A1	19960410	EP 1994-918456	19940621 <--
EP 705265	B1	19990728		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
CN 1125445	A	19960626	CN 1994-192521	19940621 <--
CN 1045778	B	19991020		
HU 74176	A2	19961128	HU 1995-3545	19940621 <--
JP 09500376	T	19970114	JP 1995-502570	19940621 <--
JP 3350550	B2	20021125		
EP 916672	A1	19990519	EP 1999-100735	19940621 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
EP 916673	A1	19990519	EP 1999-100736	19940621 <--
EP 916673	B1	20030129		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
AT 182593	T	19990815	AT 1994-918456	19940621 <--
ES 2137371	T3	19991216	ES 1994-918456	19940621 <--
NZ 328914	A	20000825	NZ 1994-328914	19940621 <--
AT 231863	T	20030215	AT 1999-100736	19940621 <--
ZA 9404463	A	19950217	ZA 1994-4463	19940622 <--
IN 177888	A1	19970222	IN 1994-CA514	19940630 <--
TW 418208	B	20010111	TW 1994-83107047	19940802 <--
IN 180930	A1	19980404	IN 1995-CA1508	19951123 <--
IN 181538	A1	19980711	IN 1995-CA1506	19951123 <--
FI 9506168	A	19960201	FI 1995-6168	19951221 <--
NO 9505219	A	19960222	NO 1995-5219	19951221 <--
BG 62933	B1	20001130	BG 1995-100258	19951227 <--
US 5939422	A	19990817	US 1996-578580	19960408 <--
US 6310205	B1	20011030	US 1999-237638	19990126 <--
US 6294541	B1	20010925	US 1999-418330	19991014 <--
US 6319928	B1	20011120	US 1999-418331	19991014 <--
PRIORITY APPLN. INFO.:			GB 1993-12853	A 19930622 <--
			EP 1994-918456	A3 19940621 <--
			NZ 1994-267468	A1 19940621 <--
			WO 1994-GB1334	W 19940621 <--
			IN 1994-CA514	A1 19940630 <--
			US 1996-578580	A2 19960408 <--
			US 1996-659767	A1 19960606 <--
			US 1997-69371P	P 19971212 <--
			US 1998-200615	B2 19981130 <--
			US 1998-210556	A2 19981211 <--
			US 1999-285473	A1 19990402 <--

OTHER SOURCE(S): MARPAT 122:239459

ED Entered STN: 18 Apr 1995

GI



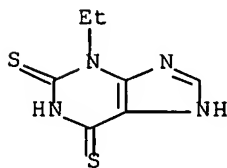
AB Title compds. [e.g., I; R1-R3, R8 = H, (cyclo)alkyl, (hetero)aryl, etc.; NR1R2 = heterocyclyl] were prepared. Title compds. have bronchial and tracheal relaxation and/or antiinflammatory activity. Thus, isovanillin was converted in 5 steps to 3,4-(HO)(MeO)C6H3CH2NHCSNH2 which was cyclocondensed with NCCH2CO2Et to give thiouracil II. The latter was converted in 3 steps to 6-amino-1-(3-cyclopentyloxy-4-methoxybenzyl)-5-isobutyrylamino-2-thiouracil which was cyclized and the product converted in 4 steps to I.HCl (R1 = Et, R2 = H, R3 = 3-cyclopentyloxy-4-methoxybenzyl, R8 = CHMe2) (III). III gave 64% inhibition of ovalbumin-induced bronchoalveolar eosinophil production in guinea pigs at 5mg/kg i.p.

IT 162278-87-7P 162278-88-8P 162278-89-9P  
 162278-90-2P 162278-91-3P 162278-93-5P  
 162278-94-6P 162279-01-8P 162279-02-9P  
 162279-04-1P 162279-05-2P 162279-06-3P  
 162279-07-4P 162279-08-5P 162279-09-6P  
 162279-10-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of purines, isoguanines, and dithioxanthines as phosphodiesterase-IV inhibitors)

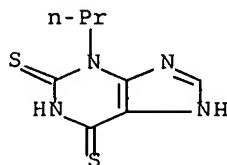
RN 162278-87-7 CAPLUS

CN 1H-Purine-2,6-dithione, 3-ethyl-3,7-dihydro- (9CI) (CA INDEX NAME)

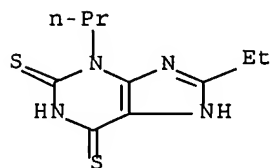


RN 162278-88-8 CAPLUS

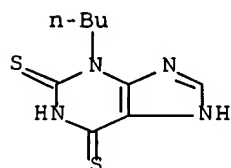
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-propyl- (9CI) (CA INDEX NAME)



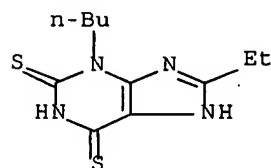
RN 162278-89-9 CAPLUS  
 CN 1H-Purine-2,6-dithione, 8-ethyl-3,7-dihydro-3-propyl- (9CI) (CA INDEX NAME)



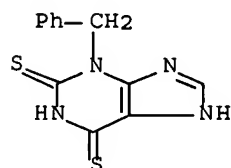
RN 162278-90-2 CAPLUS  
 CN 1H-Purine-2,6-dithione, 3-butyl-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 162278-91-3 CAPLUS  
 CN 1H-Purine-2,6-dithione, 3-butyl-8-ethyl-3,7-dihydro- (9CI) (CA INDEX NAME)

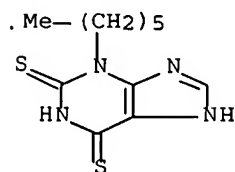


RN 162278-93-5 CAPLUS  
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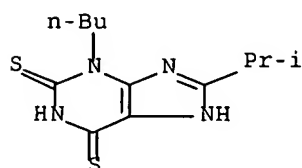
RN 162278-94-6 CAPLUS

CN 1H-Purine-2,6-dithione, 3-hexyl-3,7-dihydro- (9CI) (CA INDEX NAME)



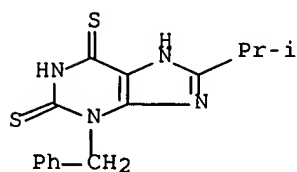
RN 162279-01-8 CAPLUS

CN 1H-Purine-2,6-dithione, 3-butyl-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



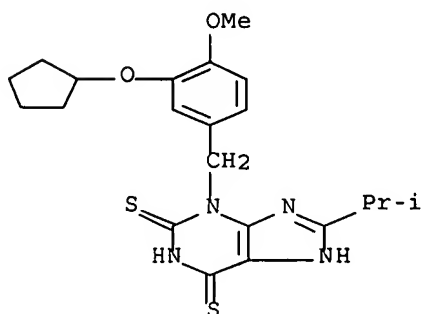
RN 162279-02-9 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 162279-04-1 CAPLUS

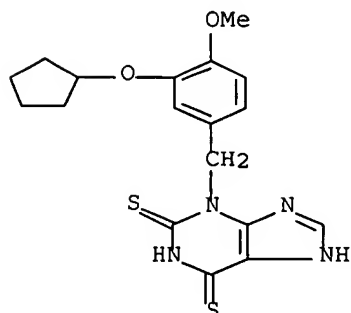
CN 1H-Purine-2,6-dithione, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)





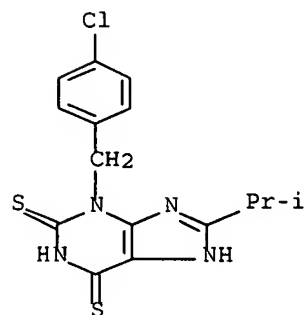
RN 162279-05-2 CAPLUS

CN 1H-Purine-2,6-dithione, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro- (9CI) (CA INDEX NAME)



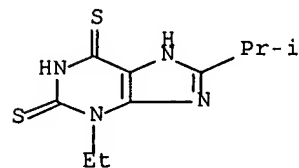
RN 162279-06-3 CAPLUS

CN 1H-Purine-2,6-dithione, 3-[(4-chlorophenyl)methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



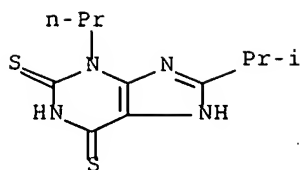
RN 162279-07-4 CAPLUS

CN 1H-Purine-2,6-dithione, 3-ethyl-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



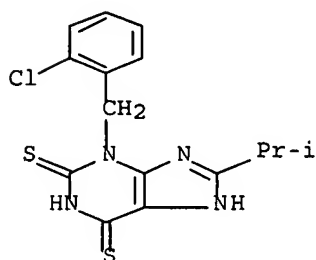
RN 162279-08-5 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-propyl- (9CI) (CA INDEX NAME)



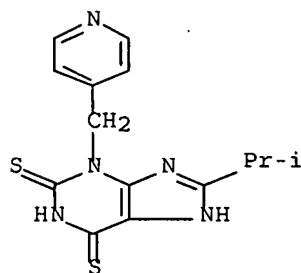
RN 162279-09-6 CAPLUS

CN 1H-Purine-2,6-dithione, 3-[(2-chlorophenyl)methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 162279-10-9 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

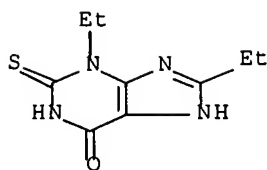


IT 162278-04-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of purines, isoguanines, and dithioxanthines as  
phosphodiesterase-IV inhibitors)

RN 162278-04-8 CAPLUS

CN 6H-Purin-6-one, 3,8-diethyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)

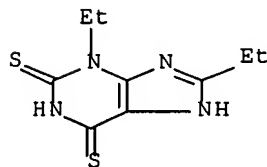


IT 162278-92-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of purines, isoguanines, and dithioxanthines as  
phosphodiesterase-IV inhibitors)

RN 162278-92-4 CAPLUS

CN 1H-Purine-2,6-dithione, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



L57 ANSWER 25 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:462796 CAPLUS Full-text

DOCUMENT NUMBER: 122:278022

TITLE: Image formation of silver halide photographic materials

INVENTOR(S): Ito, Katsuhiko; Sanpei, Takeshi

PATENT ASSIGNEE(S): Konishiroku Photo Ind, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 27 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 06347954	A	19941222	JP 1993-140638	19930611 <--
PRIORITY APPLN. INFO.:			JP 1993-140638	19930611 <--
ED Entered STN: 01 Apr 1995				
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title photog. materials, possessing  $\geq 1$  Ag halide emulsion layer on a support and containing a hydrazine derivative ANA1NA2GR [A = aryl, heterocycle containing  $\geq 1$  S or O; G = (CO)n, sulfonyl, sulfoxy, P(:O)R1, iminomethylene; n = 1, 2; A1 = A2 = H or when 1 of A1 or A2 is H the other is (substituted) alkylsulfonyl (substituted) acyl; R = H, alkyl, aryl, heterocycle, amino, OR2;

R1 = alkyl, alkenyl, alkynyl, aryl, saturated heterocycle, OR3; R2, R3 = alkyl, alkenyl, alkynyl, aryl, saturated heterocycle], an amine compound R71R72NR73 (R71-73 = H, substituent, R71-73 may form a ring), and an alc. compound R91R92CHOH (R91, R92 = H, substituent) in the emulsion layer and/or other hydrophilic colloid layer, are processed with a developing solution of pH 9.5-12.3 containing dihydroxybenzene-type developing agents, 3-pyrazolidone-type or aminophenol-type developing agents,  $\geq 0.3$  mol/L sulfites, and a N-containing heterocyclic compound selected from I, II, and III [R31-34, R41-44, R51-54 = H, SM1, OH, (substituted) alkyl, alkoxy, amino, aryl, SO3M2, CO2M3,  $\geq 1$  of R31-34,  $\geq 1$  of R41-44, and  $\geq 1$  of R51-54 are SM1; M1-3 = H, alkali metal, ammonium]. Even if the materials are processed with developing solns. containing high concns. of sulfites, Ag sludge formation is suppressed and super-high contrast images with high sensitivity are obtained. Thus, a photog. film with a Ag(Cl, I, Br) emulsion layer containing IV and Et2N(CH2)2(OCHMeCH2)7S(CH2)2NEt2 was exposed using a HeNe laser and developed with a developing solution (pH 11.5) containing hydroquinone, 4-methyl-4-hydroxymethyl-1-phenyl-3-pyrazolidone, Na2SO3 (55 g/L), and I (R31 = SH, R32-34 = H).

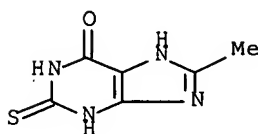
IT 91184-09-7

RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)

(hydroquinone-type photog. developer containing nitrogen-containing heterocyclic compound)

RN 91184-09-7 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-8-methyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 26 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:255796 CAPLUS Full-text

DOCUMENT NUMBER: 122:118847

TITLE: Method of processing silver halide photographic material containing hydrazine with amine-containing developer solution

INVENTOR(S): Kato, Mariko; Ishikawa, Wataru; Sanpei, Takeshi

PATENT ASSIGNEE(S): Konishiroku Photo Ind, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 31 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06250348	A	19940909	JP 1993-36906	19930225 <--
PRIORITY APPLN. INFO.:			JP 1993-36906	19930225 <--

ED Entered STN: 21 Dec 1994

AB The claimed method comprises using a developer solution consisting of (1) dihydroxybenzene, (2) derivative of 3-pyrazolidone or aminophenol, (3)  $\geq 0.3$

mol/L of sulfite, (4) amine compound R1R2CHANR3R4 and R3R4NANR5R6 (R1 = H, OH, carboxy; R2, R3, R4, R5, R6 = H, monovalent organic group; A = bivalent group; when R3 and R4 are Et, R1 ≠ OH; R3 and R5, and R4 and R6 may be combined to form heterocyclic rings), and (5) a mercapto or thion-substituted N-containing heterocyclic compd having no benzo form condensed ring. The developer solution does not generate silver sludge and reduces black peppers. It has high speed and good stability and provides high contrast images.

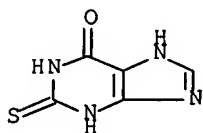
IT 2487-40-3 91184-09-7

RL: MOA (Modifier or additive use); NUU (Other use, unclassified); USES (Uses)

(photog. developer containing amine and sulfur-containing azocyclic compound)

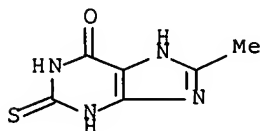
RN 2487-40-3 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



RN 91184-09-7 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-8-methyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 27 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:168945 CAPLUS Full-text

DOCUMENT NUMBER: 122:315012

TITLE: Selective Ligands for Rat A3 Adenosine Receptors: Structure-Activity Relationships of 1,3-Dialkylxanthine 7-Riboside Derivatives

AUTHOR(S): Kim, Hea Ok; Ji, Xiao-duo; Melman, Neli; Olah, Mark E.; Stiles, Gary L.; Jacobson, Kenneth A.

CORPORATE SOURCE: Laboratory of Bioorganic Chemistry, National Institute of Diabetes and Digestive and Kidney Diseases, Bethesda, MD, 20892, USA

SOURCE: Journal of Medicinal Chemistry (1994), 37(23), 4020-30

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 08 Nov 1994

AB 1,3-Dialkylxanthine 7-ribose analogs modified at the 1-, 3-, and 8-purine positions and at the ribose 5'-position were synthesized. The nucleoside analogs were examined for affinity in radioligand binding essays at rat brain A3 adenosine receptors stably expressed in CHO cells, using the radioligand

[[125I]-4-amino-3-iodobenzyl]adenosine-5'-N-methyluronamide (AB-MECA). The affinity of xanthine 7-ribosides at A3 receptors depended on the 1,3-dialkyl substituents in the order: Pent ≥ Bu » Hx > Pr ≈ Me. 1,3-Dipentylxanthine-7-riboside was slightly selective for A3 receptors (2-fold vs A1 and 10-fold vs A2a). 8-Methoxy substitution was tolerated at A3 receptors. 2-Thio vs 2-oxo substitution increased potency at all three subtypes and slightly increased A3 vs A1 selectivity. The 5'-uronamide modification, which was previously found to enhance A3 selectivity in N6-benzyladenosine derivs., was also incorporated into the xanthine 7-ribosides, with similar results. 1,3-Dibutylxanthine 7-riboside 5'-N-methylcarboxamide, with a  $K_i$  value of 229 nM at A3 receptors, was 160-fold selective for rat A3 vs A1 receptors and >400-fold selective vs A2a receptors. This derivative acted as a full agonist in the A3 receptor-mediated activation of adenylate cyclase.

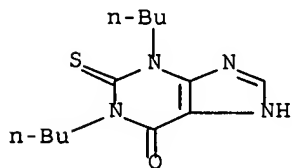
IT 77038-96-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of dialkylxanthine ribosides as selective ligands for A3 adenosine receptors)

RN 77038-96-1 CAPLUS

CN 6H-Purin-6-one, 1,3-dibutyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 28 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:500054 CAPLUS Full-text

DOCUMENT NUMBER: 121:100054

TITLE: A binding site model and structure-activity relationships for the rat A3 adenosine receptor

AUTHOR(S): van Galen, Philip J. M.; van Bergen, Andrew H.; Gallo-Rodriguez, Carola; Melman, Neli; Olah, Mark E.; Ijzerman, Ad P.; Stiles, Gary L.; Jacobson, Kenneth A.

CORPORATE SOURCE: Lab. Bioorganic Chem., Natl. Inst. Diabetes, Digestive and Kidney Diseases, Bethesda, MD, 20892, USA

SOURCE: Molecular Pharmacology (1994), 45(6), 1101-11

CODEN: MOPMA3; ISSN: 0026-895X

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 03 Sep 1994

AB A novel adenosine receptor, the A3 receptor, has recently been cloned. The authors have systematically investigated the hitherto largely unexplored structure-activity relationships (SARs) for binding at A3 receptors, using 125I-N6-2-(4-aminophenyl)ethyladenosine as a radioligand and membranes from Chinese hamster ovary cells stably transfected with the rat A3-cDNA. As is the case for A1 and A2a receptors, substitutions at the N6 and 5' positions of adenosine, the prototypic agonist ligand, may yield fairly potent compds. However, the highest affinity and A3 selectivity is found for N6,5'-disubstituted compds., in contrast to A2 and A2a receptors. Thus, N6-benzyladenosine-5'-N-ethylcarboxamide is highly potent ( $K_i$ , 6.8 nM) and moderately selective (13- and 14-fold vs. A1 and A2a). The N6 region of the

A3 receptor also appears to tolerate hydrophilic substitutions, in sharp contrast to the other subtypes. Potencies of N6,5'-disubstituted compds. in inhibition of adenylate cyclase via A3 receptors parallel their high affinity in the binding assay. None of the typical xanthine or nonxanthine (A1/A2) antagonists tested show any appreciable affinity for rat A3 receptors. 1,3-Dialkylxanthines did not antagonize the A3 agonist-induced inhibition of adenylate cyclase. A His residue in helix 6 that is absent in A3 receptors but present in A1/A2 receptors may be causal in this respect. In a mol. model for the rat A3 receptor, this mutation, together with an increased bulkiness of residues surrounding the ligand, make antagonist binding unfavorable when compared with a previously developed A1 receptor model. Second, this A3 receptor model predicted similarities with A1 and A2 receptors in the binding requirements for the ribose moiety and that xanthine-7-ribosides would bind to rat A3 receptors. This hypothesis was supported exptl. by the moderate affinity ( $K_i$ , 6  $\mu$ M) of 7-riboside of 1,3-dibutylxanthine, which appears to be a partial agonist at rat A3 receptors. The model presented here which is consistent with the detailed SAR found in this study, may serve to suggest future chemical modification, site-directed mutagenesis, and SAR studies to further define essential characteristics of the ligand-receptor interaction and to develop even more potent and selective A3 receptor ligands.

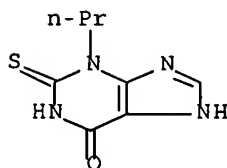
IT 156733-29-8

RL: BIOL (Biological study)

(adenosine A1 and A2a and A3 receptors affinity for, mol. structure in relation to)

RN 156733-29-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-propyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 29 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:323047 CAPLUS Full-text

DOCUMENT NUMBER: 120:323047

TITLE: Reactions of 6-thiotheophylline with alkylating agents and epichlorohydrin: isolation of S-alkylated 6-thiotheophylline and 7-(2,3-thioepoxypropyl)theophylline

AUTHOR(S): Hayashi, Hiroaki; Suzuki, Fumio; Yasuzawa, Toru; Ueno, Hideo

CORPORATE SOURCE: Pharm. Res. Lab., Kyowa Hakko Kogyo Co., Ltd., Nagaizumi, 411, Japan

SOURCE: Journal of Heterocyclic Chemistry (1993), 30(1), 247-51

CODEN: JHTCAD; ISSN: 0022-152X

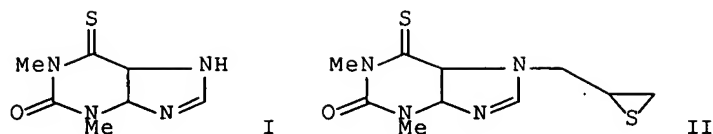
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 120:323047

ED Entered STN: 25 Jun 1994

GI



AB Alkylation of 6-thiotheophylline (I) under the aprotic basic condition affords S-alkyl-6-thiotheophylline together with an N7-alkylated product. There is a tendency that the more reactive the alkylating agents are, the higher the yields of S-alkylated products are. However, treatment of I with epichlorohydrin afforded an unexpected product, 7-(2,3-thioepoxypropyl)theophylline (II), neither an S-alkylated compound nor an N7-alkylated compound. The chemical structure was determined by NMR spectroscopic anal.

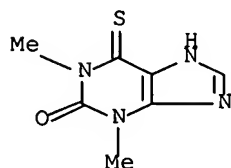
IT 2398-70-1, 6-Thiotheophylline

RL: RCT (Reactant); RACT (Reactant or reagent)

(alkylation of thiotheophylline with alkylating agents and epichlorohydrin)

RN 2398-70-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 30 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:127807 CAPLUS Full-text

DOCUMENT NUMBER: 120:127807

TITLE: Herbicidal  $\delta$ -aminolevulinic acid combinations with chlorophyll biosynthesis modulators.

INVENTOR(S): Rebeiz, Constantin A.

PATENT ASSIGNEE(S): Board of Trustees of the University of Illinois, USA

SOURCE: U.S., 40 pp. Cont.-in-part of U.S. 5,163,990.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

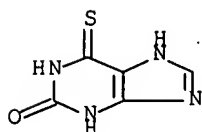
FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5242892	A	19930907	US 1990-615413	19901119 <--
EP 331211	A2	19890906	EP 1989-106579	19850717 <--
EP 331211	A3	19891123		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
ZA 8505561	A	19860326	ZA 1985-5561	19850723 <--
US 5127938	A	19920707	US 1986-895529	19860811 <--



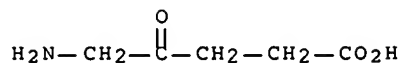
US 5200427	A	19930406	US 1989-294132	19890109 <--
US 5163990	A	19921117	US 1990-521119	19900503 <--
CA 2080140	A1	19911104	CA 1991-2080140	19910502 <--
CA 2080140	C	20020108		
WO 9116820	A1	19911114	WO 1991-US3015	19910502 <--
W: CA, JP, KR				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
EP 527186	A1	19930217	EP 1991-909022	19910502 <--
R: BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL				
JP 06500989	T	19940127	JP 1991-508902	19910502 <--
CA 2358003	C	20020924	CA 1991-2358003	19910502 <--
US 5286708	A	19940215	US 1991-773030	19911008 <--
US 5300526	A	19940405	US 1991-795367	19911120 <--
US 5321001	A	19940614	US 1992-915896	19920717 <--
JP 2001151614	A	20010605	JP 2000-226123	20000621 <--
JP 3365503	B2	20030114		
JP 2003063907	A	20030305	JP 2002-236923	20020815 <--
JP 3734780	B2	20060111		
PRIORITY APPLN. INFO.:			US 1984-634932	B2 19840727 <--
			US 1985-754092	B1 19850715 <--
			US 1986-895529	A2 19860811 <--
			US 1990-521119	A2 19900503 <--
			EP 1985-903637	P 19850717 <--
			US 1988-144883	B2 19880113 <--
			US 1989-294132	A3 19890109 <--
			US 1990-615413	A 19901119 <--
			CA 1991-2080140	A3 19910502 <--
			JP 1991-508902	A3 19910502 <--
			WO 1991-US3015	W 19910502 <--
			JP 2000-226123	A3 20000621 <--
ED	Entered STN: 19 Mar 1994			
AB	The title compns. are defoliants and herbicides, with activity based on the accumulation of photodynamic tetrapyrrols. A mixture of 20 mM $\gamma$ -aminolevulinic acid and 15 mM 6-aminonicotinic acid defoliated tomato seedlings.			
IT	152968-88-2			
	RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)			
	(herbicide and defoliant)			
RN	152968-88-2 CAPLUS			
CN	Pentanoic acid, 5-amino-4-oxo-, mixt. with 1,3,6,7-tetrahydro-6-thioxo-2H-purin-2-one (9CI) (CA INDEX NAME)			
CM	1			
CRN	2002-59-7			
CMF	C5 H4 N4 O S			



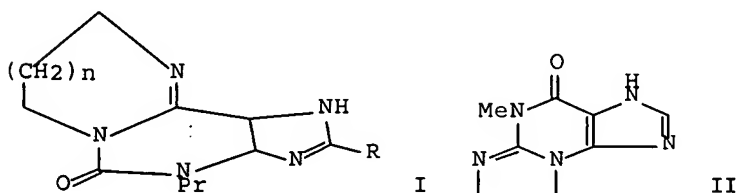
CM 2

CRN 106-60-5

CMF C5 H9 N O3



L57 ANSWER 31 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1994:77080 CAPLUS Full-text  
 DOCUMENT NUMBER: 120:77080  
 TITLE: Convenient synthesis of tricyclic purine derivatives  
 AUTHOR(S): Shimada, Junichi; Kuroda, Takeshi; Suzuki, Fumio  
 CORPORATE SOURCE: Pharm. Res. Lab., Kyowa Hakko Kogyo Co., Ltd.,  
 Shizuoka, 411, Japan  
 SOURCE: Journal of Heterocyclic Chemistry (1993),  
 30(1), 241-6  
 CODEN: JHTCAD; ISSN: 0022-152X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 120:77080  
 ED Entered STN: 19 Feb 1994  
 GI

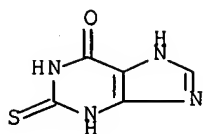


AB A convenient synthesis of the title compds. I (R = H, cyclopentyl; n = 0-2) and II is described. The syntheses of I and II were accomplished by treatment of 6-methylthio-7H-purin-2(3H)-ones or 2-benzylthio-1-methyl-9-triphenylmethyl-9H-purin-6(1H)-one (III) with the appropriate amino alc. followed by dehydrative cyclization using SOCl<sub>2</sub>. III was efficiently prepared by benzylation of 6-hydroxy-2-mercaptapurine followed by tritylation and N-methylation.

IT 2487-40-3, 6-Hydroxy-2-mercaptapurine  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (benzylation of)

RN 2487-40-3 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)

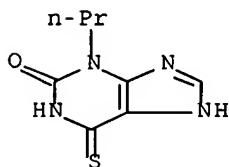


IT 105396-65-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
(methylation of)

RN 105396-65-4 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 32 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:644995 CAPLUS Full-text

DOCUMENT NUMBER: 117:244995

TITLE: Approach to an adenosine pharmacophore by molecular modeling

AUTHOR(S): Neuwels, M.

CORPORATE SOURCE: UCB Sect. Pharm., Chemin Foriest, Braine-l-Alleud, B-1420, Belg.

SOURCE: Journal de Pharmacie de Belgique (1992), 47(4), 351-63

CODEN: JPBEAJ; ISSN: 0047-2166

DOCUMENT TYPE: Journal

LANGUAGE: French

ED Entered STN: 26 Dec 1992

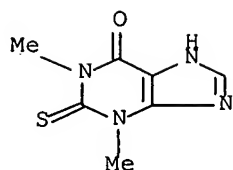
AB The selective development of adenosine A1 antagonists was carried out in 2 steps. First an A1 pharmacophore common to various known chemical families was determined in order to permit the design of new chemical skeletons; then a predictive modeling of affinities was carried out to select new potential ligands. The mol. modeling was done on 6 different chemical families (triazoloquinoxalines, adenines, xanthines, pyrazolopyrimidinones, triazoloquinazolines, and imidazoquinolines), and a search for a common superimposition was carried out. Starting from the different superpositions obtained, a CoMFA study (QSAR-3D) allowed the building of predictive models for A1 receptor affinity. The theor. preferred superposition proved to be the best, as it was able to correctly predict the activities of new ligands.

IT 6603-63-0

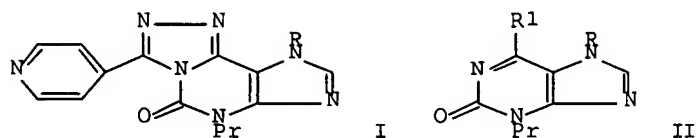
RL: BIOL (Biological study)  
(in mol. modeling of adenosine receptor pharmacophore)

RN 6603-63-0 CAPLUS

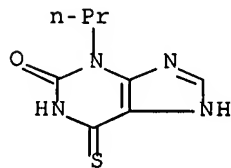
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 33 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1992:469819 CAPLUS Full-text  
 DOCUMENT NUMBER: 117:69819  
 TITLE: Facile synthesis of 9H-s-triazolo[3,4-i]purin-5(6H)-ones  
 AUTHOR(S): Shimada, Junichi; Suzuki, Fumio  
 CORPORATE SOURCE: Pharm. Res. Lab., Kyowa Hakko Kogyo Co., Ltd., Shizuoka, 411, Japan  
 SOURCE: Tetrahedron Letters (1992), 33(22), 3151-4  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 117:69819  
 ED Entered STN: 23 Aug 1992  
 GI

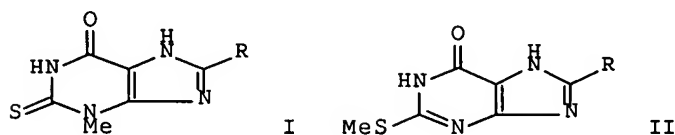


AB New tricyclic heterocycles, 9H-s-triazolo[3,4-i]purin-5(6H)-ones I (R = Me, H), were prepared from 6-methylthio-7H-purin-2(3H)-ones II (R = Me, PhCH<sub>2</sub>OCH<sub>2</sub>; R<sub>1</sub> = MeS) via cyclization of II (R<sub>1</sub> = isonicotinoylhydrazino).  
 IT 105396-65-4, 3-Propyl-6-thioxanthine  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (methylation or benzylation of)  
 RN 105396-65-4 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 34 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1992:426495 CAPLUS Full-text

DOCUMENT NUMBER: 117:26495  
 TITLE: Facile and general synthesis of 8-substituted  
 2-(methylthio)purin-6-ones  
 AUTHOR(S): Nagamatsu, Tomohisa; Yamasaki, Hiroo  
 CORPORATE SOURCE: Fac. Pharm. Sci., Okayama Univ., Tsushima, 700, Japan  
 SOURCE: Heterocycles (1992), 33(2), 775-90  
 CODEN: HTCYAM; ISSN: 0385-5414  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 117:26495  
 ED Entered STN: 26 Jul 1992  
 GI



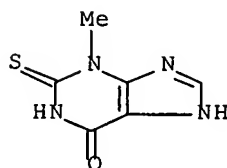
AB 3-Methyl-6-oxo-2-thioxo-1,2,3,6-tetrahydropurines [I; R = H, alkyl, (un)substituted Ph] were synthesized by oxidative cyclization of 5,6-diamino-1-methyl-2-thiouracil-RCHO reaction products or 6-amino-5-(benzylideneamino)-1-methyl-2-thiouracils in the presence of di-Et azodicarboxylate (DEAD). In addition, the oxidative cyclization of 4-amino-5-(benzylideneamino)-3-methyl-2-(methylthio)pyrimidin-6(3H)-ones in the presence of DEAD gave 8-aryl-3-methyl-2-(methylthio)-6-oxo-3,6-dihydropurines, which were identical with the compds. prepared by methylation of I. 2-(Methylthio)-6-oxo-1,6-dihydropurines [II; R = H, alkyl, (un)substituted Ph] were synthesized from 4,5-diamino-2-(methylthio)pyrimidin-6(1H)-one or 4-amino-5-(benzylideneamino)-2-(methylthio)pyrimidin-6(1H)-ones in a similar manner as above.

IT 28139-02-8P 91725-06-3P 103289-69-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and methylation of)

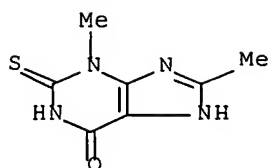
RN 28139-02-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)

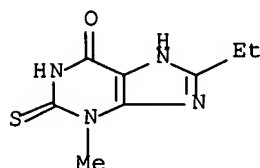


RN 91725-06-3 CAPLUS

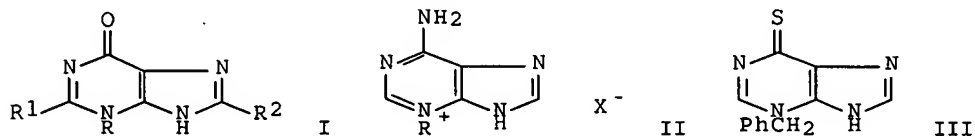
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3,8-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 103289-69-6 CAPLUS  
 CN 6H-Purin-6-one, 8-ethyl-1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 35 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1992:214213 CAPLUS Full-text  
 DOCUMENT NUMBER: 116:214213  
 TITLE: Inhibitors of human purine nucleoside phosphorylase.  
 Synthesis and biological activities of  
 8-amino-3-benzylhypoxanthine and related analogs  
 AUTHOR(S): Woo, Peter W. K.; Kostlan, Catherine R.; Sircar,  
 Jagadish C.; Dong, Mi K.; Gilbertsen, Richard B.  
 CORPORATE SOURCE: Parke-Davis Pharm. Res. Div., Warner-Lambert Co., Ann  
 Arbor, MI, 48105, USA  
 SOURCE: Journal of Medicinal Chemistry (1992),  
 35(8), 1451-7  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 116:214213  
 ED Entered STN: 31 May 1992  
 GI



AB 3-Substituted hypoxanthines I (R = CH<sub>2</sub>Ph, CH<sub>2</sub>C<sub>6</sub>H<sub>3</sub>Cl<sub>2</sub>-3,4, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>CN-4, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>-4, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>OMe-4, CH<sub>2</sub>CH<sub>2</sub>Ph, 2-thienylmethyl, 2-furylmethyl; R<sub>1</sub> = H, SMe, OH, NH<sub>2</sub>; R<sub>2</sub> = H, NH<sub>2</sub>; NHCHO) and analogs II (R = CH<sub>2</sub>Ph, X = Cl; R = CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>-4, X = Br) and III have been synthesized as inhibitors of purine nucleoside phosphorylase (PNP), which may conceivably act as T-cell-selective immunosuppressive agents with potential utility in autoimmune disorders such

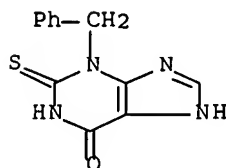
as rheumatoid arthritis, in organ transplantations, and in T-cell leukemias. The compds. were evaluated for their PNP activity by a radiochem. assay and also for their cytotoxic effects on a T-lymphoblastoid cell line (MOLT-4). Appropriate substitutions on 3-benzylhypoxanthine (I, R = CH<sub>2</sub>Ph, R<sub>1</sub>, R<sub>2</sub> = H) increase potency. Variation of the 3-aryl substituents of I (R = CH<sub>2</sub>Ph, R<sub>1</sub>, R<sub>2</sub> = H) failed to further increase potency. Replacement of the 6-oxygen function in I (R = CH<sub>2</sub>Ph, R<sub>1</sub>, R<sub>2</sub> = H) to give II or III resulted in little change in activity. Other variations resulted in decreased activity. I (R = CH<sub>2</sub>Ph, 2-thienylmethyl, 2-furylmethyl, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>OMe-4, R<sub>1</sub>, R<sub>2</sub> = NH<sub>2</sub>) have moderate but significant activities, as compared to the most active inhibitor presently known, 8-amino-9-thienylguanine. I (R<sub>1</sub>, R<sub>2</sub> = NH<sub>2</sub>) represent a novel structural type which were prepared via formation of the aminoimidazole moiety through a base-catalyzed 1,5-(O → N)-carbamimidoyl rearrangement.

IT 28741-76-6P 139460-82-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, reductive dethiolation, and purine nucleoside  
phosphorylase-inhibiting activity of)

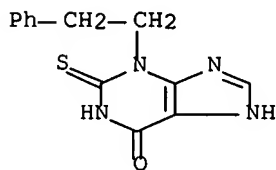
RN 28741-76-6 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-(phenylmethyl)-2-thioxo- (9CI) (CA  
INDEX NAME)



RN 139460-82-5 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-(2-phenylethyl)-2-thioxo- (9CI) (CA  
INDEX NAME)



L57 ANSWER 36 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:582959 CAPLUS Full-text

DOCUMENT NUMBER: 115:182959

TITLE: Preparation of xanthine derivatives as angiotensin II  
antagonists

INVENTOR(S): Morimoto, Akira; Nishikawa, Kohei

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: Eur. Pat. Appl., 38 pp.

CODEN: EPXXDW

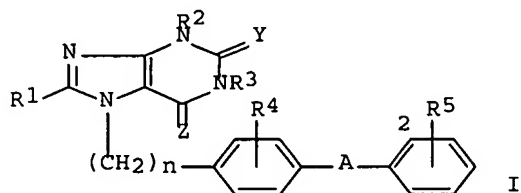
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 430300	A2	19910605	EP 1990-123013	19901130 <--
EP 430300	A3	19920325		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 03223284	A	19911002	JP 1990-338861	19901130 <--
CA 2031328	A1	19910602	CA 1990-2031328	19901203 <--
PRIORITY APPLN. INFO.:			JP 1989-313918	A 19891201 <--
OTHER SOURCE(S):			MARPAT 115:182959	
ED Entered STN: 01 Nov 1991				
GI				



AB Xanthine derivs. [I; R1 = (substituted) hydrocarbyl, optionally bound through a hetero atom; one of R2 and R3 = (substituted) hydrocarbyl, the other is H or (substituted) hydrocarbyl; R4 = H, halo, NO2; R5 = a group capable of forming an anion; A = bond, a spacer having atomic length  $\leq 2$ ; n = 1, 2; Y, Z = O, S], useful in treating hypertension, heart diseases, strokes, etc., are prepared To a solution of cyano compound I (R1 = Bu, R2 = R3 = Me, R4 = H, R5 = 2-cyano, A = bond, Y = Z = O, n = 1) in DMF were added NaN<sub>3</sub> and NH<sub>4</sub>Cl with stirring at 115° to give 59.8% tetrazole derivative I [R1 = Bu, R2 = R3 = Me, R4 = H, R5 = 2-(1H-tetraol-5-yl), A = bond, Y = Z = O, n = 1], which showed IC<sub>50</sub> of  $2.8 \times 10^{-7}$  M against angiotensin II binding. Capsule, tablet, and injection formulations were given.

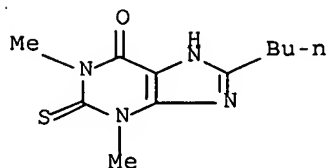
IT 136420-18-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of angiotensin II antagonist)

RN 136420-18-3 CAPLUS

CN 6H-Purin-6-one, 8-butyl-1,2,3,7-tetrahydro-1,3-dimethyl-2-thiooxo- (9CI)  
(CA INDEX NAME)



L57 ANSWER 37 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:536115 CAPLUS Full-text

DOCUMENT NUMBER: 115:136115

TITLE: Preparation of condensed purine derivatives as drugs

INVENTOR(S): Suzuki, Fumio; Shimada, Junichi; Kuroda, Takeshi;



Kubo, Kazuhiro; Karasawa, Akira; Ohno, Tetsuji;  
Ohmori, Kenji  
PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan  
SOURCE: Eur. Pat. Appl., 43 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 423805	A2	19910424	EP 1990-120056	19901019 <--
EP 423805	A3	19920102		
EP 423805	B1	20000823		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
CA 2028235	A1	19910421	CA 1990-2028235	19901019 <--
CA 2028235	C	19970121		
JP 03204880	A	19910906	JP 1990-281578	19901019 <--
US 5270316	A	19931214	US 1990-599758	19901019 <--
AT 195739	T	20000915	AT 1990-120056	19901019 <--
ES 2152207	T3	20010201	ES 1990-120056	19901019 <--
			JP 1989-273403	A 19891020 <--

PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 115:136115

ED Entered STN: 05 Oct 1991

GI For diagram(s), see printed CA Issue.

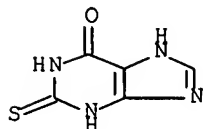
AB Title compds. I (A = Q, Q1, Q2; R1 = H, alkyl, alicyclic alkyl, noradamantan-3-yl, dicyclopropylmethyl, styryl; R2 = H, alkyl, alicyclic alkyl; R3 = H, alkyl, PhCH2; X1, X2 = H, alkyl, aralkyl, Ph; n = 0, 1) or a salt thereof, useful as diuretics, renal protecting agents, bronchodilators or hypotensives, are prepared Thus, H2NCH2CH2OH was added to 3,7-dihydro-7-methyl-6-(methylthio)-3-propyl-2H-purin-2-one (preparation given) and treated at 160° for 1 h to give the hydroxyethylamino derivative which was refluxed with POCl3 and after workup to give the imidazaopurinone II. II showed biol. activity as the above agents. Pharmaceutical formulations are given.

IT 2487-40-3, 2-Mercapto-6-hydroxypurine

RL: RCT (Reactant); RACT (Reactant or reagent)  
(benzylation of)

RN 2487-40-3 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)

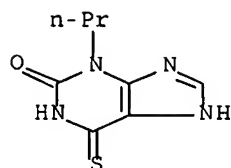


IT 105396-65-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
(methylation of)

RN 105396-65-4 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



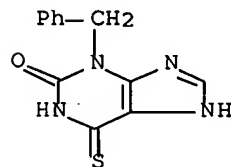
IT 19844-94-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of condensed purines as drugs)

RN 19844-94-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(phenylmethyl)-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 38 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:491963 CAPLUS Full-text

DOCUMENT NUMBER: 115:91963

TITLE: Preparation and formulation of s-triazolo[3,4-i]purine derivatives as bronchodilators, diuretics, renal protectants, and antiamnesic agents

INVENTOR(S): Suzuki, Fumio; Shimada, Junichi; Ohmori, Kenji; Manabe, Haruhiko; Kubo, Kazuhiro; Karasawa, Akira; Ohno, Tetsuji; Shiozaki, Shizuo; Ishii, Akio; Shuto, Katsuichi

PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 52 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 417790	A2	19910320	EP 1990-117662	19900913 <--
EP 417790	A3	19920318		
EP 417790	B1	19961204		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 03204879	A	19910906	JP 1990-243248	19900913 <--
JP 2980658	B2	19991122		
AT 145908	T	19961215	AT 1990-117662	19900913 <--
ES 2097124	T3	19970401	ES 1990-117662	19900913 <--
CA 2025413	A1	19910315	CA 1990-2025413	19900914 <--
CA 2025413	C	19971104		
US 5173492	A	19921222	US 1991-752180	19910823 <--

PRIORITY APPLN. INFO.:

JP 1989-239117

A 19890914 &lt;--

JP 1989-261761

A 19891006 &lt;--

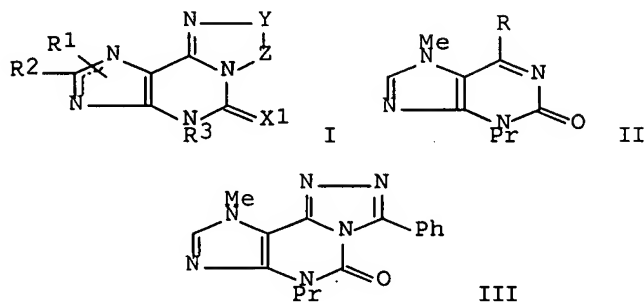
US 1990-581562

B1 19900912 &lt;--

OTHER SOURCE(S): MARPAT 115:91963

ED Entered STN: 06 Sep 1991

GI



AB The title compds. [I; R1, R2 = H, alkyl, cycloalkyl, aralkyl, (substituted) aryl; R3 = alkyl, cycloalkyl, aralkyl, (substituted) aryl; X1 = O, S; YZ = N:CR4 or NR4C(:X2) wherein R4 = H, alkyl, (substituted) (hetero)aryl, X2 = O, S, NH] are prepared PhCONHNH2 was added to a suspension of II (R = MeS) (preparation given) in MePh, the mixture was refluxed to give 60% hydrazine derivative II (R = PhCONHNH), which (2.64 g) was refluxed with 308 mg p-MeC6H4SO3H in MePh to give 67% title compound III. III showed IC50 of 4.1  $\mu$ M in passive Schultz-Dale reaction (bronchodilatory effects) and diuretic activity at 25 mg/kg orally in rats. Also prepared and tested were 50 addnl. I. Tablet, syrup, powder, and capsule formulations were also given.

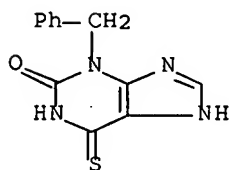
IT 19844-94-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of triazolopurine drugs)

RN 19844-94-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(phenylmethyl)-6-thioxo- (9CI) (CA INDEX NAME)



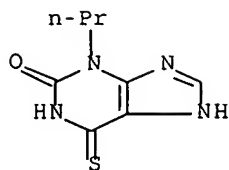
IT 105396-65-4 135445-55-5

RL: RCT (Reactant); RACT (Reactant or reagent)

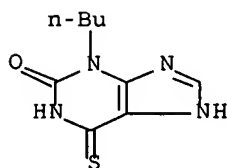
(reaction of, in preparation of triazolopurine drugs)

RN 105396-65-4 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 135445-55-5 CAPLUS  
 CN 2H-Purin-2-one, 3-butyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)

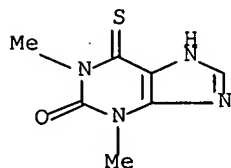


L57 ANSWER 39 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1990:111839 CAPLUS Full-text  
 DOCUMENT NUMBER: 112:111839  
 TITLE: Pharmacological effects and binding studies of new methylxanthine thioderivatives  
 AUTHOR(S): Ragazzi, E.; Frolidi, G.; Santi Soncin, E.; Borea, P. A.; Fassina, G.  
 CORPORATE SOURCE: Dep. Pharmacol., Univ. Padua, Padua, I-35131, Italy  
 SOURCE: Pharmacological Research (1989), 21(6), 707-17  
 CODEN: PHMREP; ISSN: 1043-6618  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 31 Mar 1990  
 AB The pharmacol. effects of 2 methylxanthine derivs., 6-thiocaffeine (TC) and 6-thiotheophylline (TT), were studied in different in vitro and in vivo conditions. On guinea-pig isolated trachea, both TC and TT showed a relaxant effect (EC50 50  $\mu$ M and 60  $\mu$ M, resp.), more potent than theophylline (300  $\mu$ M). In guinea-pig isolated atria, TC (30-50  $\mu$ M) antagonized N6-phenylisopropyladenosine (a stable agonist on adenosine receptors) neg. effect in not a clearly competitive way. Higher concentration (100  $\mu$ M) began to reverse that inhibitory effect. In vitro Ki of TC and TT for A1 and A2 adenosine receptors was intermediate in comparison to caffeine and theophylline. On the contrary, the 2 thioderivs. showed a higher affinity for [3H]-nitrendipine binding sites, in comparison to the original methylxanthines; this can be responsible for an antagonism at the level of Ca2+ L-type channels, at concns. <1 mM, when caffeine and theophylline are not effective. In vivo expts. in mice provided evidence for a lack of CNS stimulant effects, but a loss of motor coordination was observed Both thioderivs. showed a reduced acute toxicity.  
 IT 2398-70-1, 6-Thiotheophylline  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(pharmacol. of, mechanisms in)

RN 2398-70-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 40 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1990:55760 CAPLUS Full-text

DOCUMENT NUMBER: 112:55760

TITLE: Synthesis of new thiotheophylline azo compounds and their application as photometric reagents for vanadium(V)

AUTHOR(S): Guseinov, I. K.; Agaragimov, M. A.; Askerov, D. N.

CORPORATE SOURCE: Inst. Neorg. Fiz. Khim., Baku, USSR

SOURCE: Azerbaidzhanskii Khimicheskii Zhurnal (1988), (1), 131-7

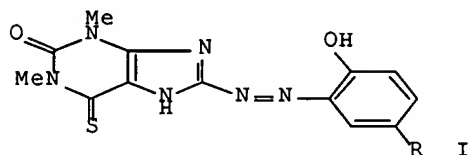
CODEN: AZKZAU; ISSN: 0005-2531

DOCUMENT TYPE: Journal

LANGUAGE: Russian

ED Entered STN: 17 Feb 1990

GI



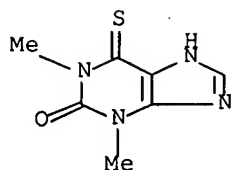
AB The title compds. I (R = H, Cl, SO<sub>3</sub>H, NO<sub>2</sub>) were prepared in 32-48% yields by coupling reactions of 6-thiotheophylline, prepared in 91% yield by sulfuration of theophylline with P<sub>2</sub>S<sub>5</sub>, with diazotized aminophenols. I are useful in photometric determination of vanadium(V).

IT 2398-70-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and coupling reaction with diazotized aminophenols)

RN 2398-70-1 CAPLUS

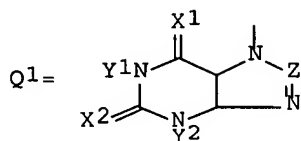
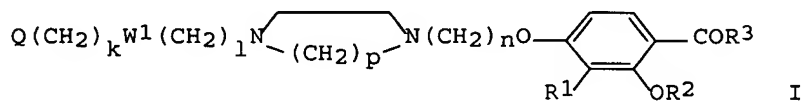
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 41 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1990:35563 CAPLUS Full-text  
 DOCUMENT NUMBER: 112:35563  
 TITLE: Preparation of xanthine derivatives as leukotriene antagonists  
 INVENTOR(S): Suzuki, Fumio; Shimada, Junichi; Hayashi, Hiroaki; Oomori, Takemori; Manabe, Haruhiko  
 PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 22 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01156978	A	19890620	JP 1988-169572	19880707 <--
PRIORITY APPLN. INFO.: MARPAT 112:35563			JP 1987-239270	A1 19870924 <--

OTHER SOURCE(S):  
 ED Entered STN: 04 Feb 1990  
 GI



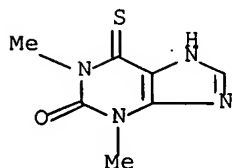
AB The title compds. I [Q = xanthine, 8-azaxanthine residue (e.g., Q1, etc.); Z = N, CY3; Y1-Y3 = H, alkyl, alkenyl, etc.; X1, X2 = O, S; W1, W2, CH2, CHOA, etc.; A = H, acyl; R1 = alkyl, alkenyl; R2 = H, acyl; R3 = H, alkyl, cycloalkyl; k, l, m, n = 0-4; p = 1-3] and salts thereof, useful as leukotriene antagonists, were prepared. A mixture of 1,3-dimethyl-7-(3-iodopropyl)xanthine, 2-hydroxy-3-propyl-4-[3-(1-piperazinyl)propoxy]acetophenone, and Et3N in EtOH was refluxed for 2.5 h to give, after acidification with HCl, 69% 7-[3-[4-[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]1-piperazinyl]propyl]-1,3-dimethylxanthine-3HCl (II). II exhibited an IC50 of 0.93  $\mu$ M against leukotriene D4 in a test using guinea pig tracheal strips.

IT 2398-70-1 40915-18-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, in preparation of leukotriene antagonist)

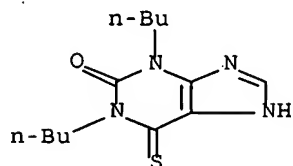
RN 2398-70-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 40915-18-2 CAPLUS

CN 2H-Purin-2-one, 1,3-dibutyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 42 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1988:542347 CAPLUS Full-text

DOCUMENT NUMBER: 109:142347

TITLE: New methylxanthine thio-derivatives inducing marked tracheal relaxation without increasing cardiac inotropism or motor activity

AUTHOR(S): Ragazzi, E.; Froidi, G.; Soncin, E. Santi; Fassina, G.

CORPORATE SOURCE: Dep. Pharmacol., Univ. Padua, Padua, Italy

SOURCE: Pharmacological Research Communications (1988), 20(7), 621-2

CODEN: PLRCAT; ISSN: 0031-6989

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 28 Oct 1988

AB The methylxanthine derivative 6-thiocaffeine at 0.01-1 mM had neg. inotropic and chronotropic effects on isolated guinea pig atria, whereas 6-thiotheophylline had neg. effects only at high concns. (>1 mM). In addition, 6-thiocaffeine at 3-100 µM increased the heart rate, did not affect contraction, and reduced perfusion pressure in isolated guinea pig hearts. Both methylxanthines relaxed the guinea pig trachea with EC50 of .apprx.50 µM. The LD50 values for 6-thiocaffeine and 6-thiotheophylline were 365 and 430 mg/kg, i.p., resp. Neither compound increased locomotor activity, and 6-thiotheophylline caused a behavioral depression.

IT 2398-70-1, 6-Thiotheophylline

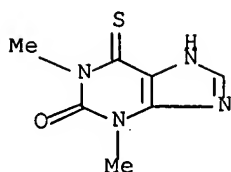
RL: PRP (Properties)

(trachea relaxation from and cardiac effects of)

RN 2398-70-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX

NAME)

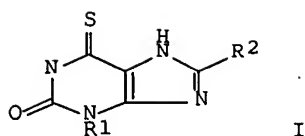


L57 ANSWER 43 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1988:406542 CAPLUS Full-text  
 DOCUMENT NUMBER: 109:6542  
 TITLE: Preparation, formulation, and testing of  
 6-thioxanthine bronchodilators  
 INVENTOR(S): Hofer, Peter  
 PATENT ASSIGNEE(S): Euro-Celtique S. A., Luxembourg  
 SOURCE: Eur. Pat. Appl., 12 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 256692	A2	19880224	EP 1987-306557	19870724 <--
EP 256692	A3	19890830		
EP 256692	B1	19920916		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
DK 8703677	A	19880203	DK 1987-3677	19870715 <--
DK 161965	B	19910902		
DK 161965	C	19920210		
ZA 8705346	A	19880330	ZA 1987-5346	19870721 <--
CA 1276147	C	19901113	CA 1987-542734	19870722 <--
AT 80632	T	19921015	AT 1987-306557	19870724 <--
ES 2046204	T3	19940201	ES 1987-306557	19870724 <--
US 4925847	A	19900515	US 1987-78545	19870728 <--
AU 8776286	A	19880204	AU 1987-76286	19870730 <--
AU 601456	B2	19900913		
JP 63041478	A	19880222	JP 1987-191515	19870730 <--
JP 2590120	B2	19970312		
US 5010081	A	19910423	US 1989-415970	19891002 <--
PRIORITY APPLN. INFO.:				
			GB 1986-18931	A 19860802 <--
			US 1985-699254	A2 19850207 <--
			EP 1987-306557	A 19870724 <--
			US 1987-78545	A1 19870728 <--
			US 1989-322364	B2 19890313 <--

OTHER SOURCE(S): MARPAT 109:6542  
 ED Entered STN: 09 Jul 1988  
 GI





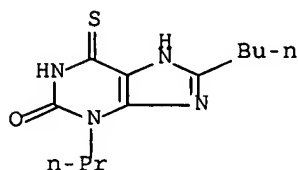
AB The title compds. (I; R1 = C2-6 alkyl, C3-7 cycloalkyl, C4-8 cycloalkylalkyl; R2 = C1-6 alkyl, C3-7 cycloalkyl, C4-8 cycloalkylalkyl; provided that when R1 = Et, Pr, or Bu, R2 = C3-6 alkyl, C3-7 cycloalkyl, or C4-8 cycloalkylalkyl) were prepared as bronchodilators. 3-Ethyl-8-butylxanthine and P2S5 were refluxed in pyridine to give 70% 3-ethyl-8-butyl-6-thioxanthine. The latter was 55.0 times as active in relaxing isolated guinea pig tracheal tissue than theophylline.

IT 114834-11-6P 114834-12-7P 114834-13-8P  
114834-14-9P 114834-17-2P 114834-18-3P  
114834-19-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as bronchodilator)

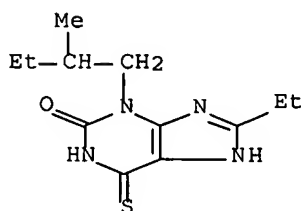
RN 114834-11-6 CAPLUS

CN 2H-Purin-2-one, 8-butyl-1,3,6,7-tetrahydro-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



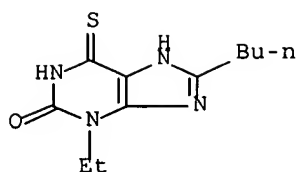
RN 114834-12-7 CAPLUS

CN 2H-Purin-2-one, 8-ethyl-1,3,6,7-tetrahydro-3-(2-methylbutyl)-6-thioxo- (9CI) (CA INDEX NAME)



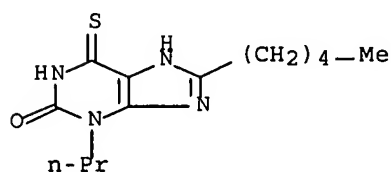
RN 114834-13-8 CAPLUS

CN 2H-Purin-2-one, 8-butyl-3-ethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



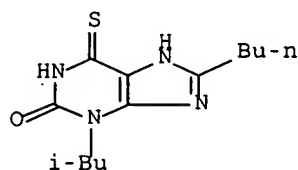
RN 114834-14-9 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-8-pentyl-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



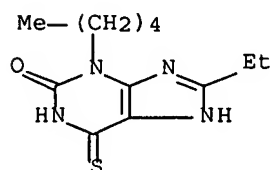
RN 114834-17-2 CAPLUS

CN 2H-Purin-2-one, 8-butyl-1,3,6,7-tetrahydro-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



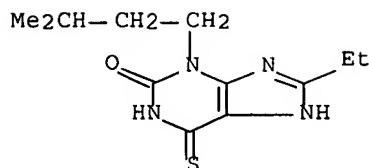
RN 114834-18-3 CAPLUS

CN 2H-Purin-2-one, 8-ethyl-1,3,6,7-tetrahydro-3-pentyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 114834-19-4 CAPLUS

CN 2H-Purin-2-one, 8-ethyl-1,3,6,7-tetrahydro-3-(3-methylbutyl)-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 44 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1988:86769 CAPLUS Full-text

DOCUMENT NUMBER: 108:86769

TITLE: The 2-thioxanthine and its chlorohydrate. Synthesis, characterization and complexing behavior with palladium(II), rhodium(III), gold(III) and platinum(IV)

AUTHOR(S): Sanchez Sanchez, M. P.; Salas Peregrin, J. M.; Romero Molina, M. A.

CORPORATE SOURCE: Fac. Cienc., Univ. Granada, Spain

SOURCE: Anales de Quimica, Serie B: Quimica Inorganica y Quimica Analitica (1987), 83(2), 129-34  
CODEN: AQSAD3; ISSN: 0211-1349

DOCUMENT TYPE: Journal

LANGUAGE: Spanish

ED Entered STN: 05 Mar 1988

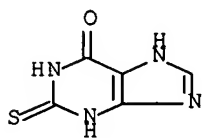
AB 2-Thioxanthine hydrochloride (TXH<sub>2</sub>Cl), Pd(TXH)<sub>2</sub>Cl<sub>2</sub>·2H<sub>2</sub>O, Rh(TX)<sub>2</sub>Cl<sub>2</sub>·3H<sub>2</sub>O, Au(TX)Cl<sub>2</sub>, and Pt(TX)<sub>2</sub>Cl<sub>2</sub>·H<sub>2</sub>O were prepared. These compds. and TXH were characterized by elemental anal. and spectral (electronic, NMR, IR) methods. The thermal decomposition of the complexes was also studied.

IT 104187-16-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and spectra of)

RN 104187-16-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo-, monohydrochloride (9CI) (CA INDEX NAME)



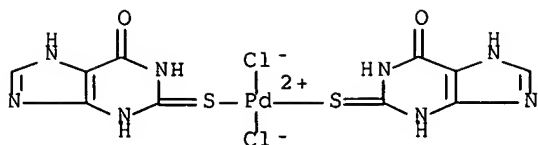
● HCl

IT 112614-64-9P

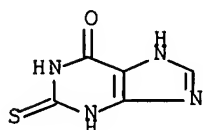
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and thermolysis and spectra of)

RN 112614-64-9 CAPLUS

CN Palladium, dichlorobis(1,2,3,7-tetrahydro-2-thioxo-6H-purin-6-one-S)-, (SP-4-1)- (9CI) (CA INDEX NAME)



IT 2487-40-3, 2-Thioxanthine  
 RL: PRP (Properties)  
 (reaction with hydrochloric acid and spectra of)  
 RN 2487-40-3 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 45 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1986:626214 CAPLUS Full-text  
 DOCUMENT NUMBER: 105:226214  
 TITLE: 6-Thioxanthine derivatives  
 INVENTOR(S): Hofer, Peter  
 PATENT ASSIGNEE(S): Euro-Celtique S. A., Luxembourg  
 SOURCE: Eur. Pat. Appl., 7 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

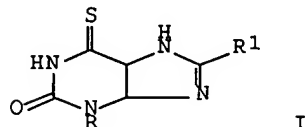
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 191313	A1	19860820	EP 1986-100544	19860117 <--
EP 191313	B1	19921028		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
US 4710503	A	19871201	US 1985-699254	19850207 <--
IN 161914	A1	19880227	IN 1985-CA906	19851218 <--
ZA 8509805	A	19860827	ZA 1985-9805	19851223 <--
IL 77430	A	19881031	IL 1985-77430	19851224 <--
AU 8651840	A	19860814	AU 1986-51840	19860103 <--
AU 570142	B2	19880303		
AT 81858	T	19921115	AT 1986-100544	19860117 <--
FI 8600285	A	19860808	FI 1986-285	19860121 <--
FI 84180	B	19910715		
FI 84180	C	19911025		
DK 8600332	A	19860808	DK 1986-332	19860122 <--
DK 161964	B	19910902		
DK 161964	C	19920210		
CN 86101050	A	19861112	CN 1986-101050	19860205 <--
CN 1013676	B	19910828		
NO 8600424	A	19860808	NO 1986-424	19860206 <--
NO 163569	B	19900312		

NO 163569	C	19900620		
CA 1275288	C	19901016	CA 1986-501288	19860206 <--
JP 61183287	A	19860815	JP 1986-24248	19860207 <--
JP 07080882	B	19950830		
US 4820709	A	19890411	US 1987-75937	19870722 <--
US 4925847	A	19900515	US 1987-78545	19870728 <--
US 5010081	A	19910423	US 1989-415970	19891002 <--
JP 08099882	A	19960416	JP 1995-6756	19950119 <--
JP 2888273	B2	19990510		

PRIORITY APPLN. INFO.:

	US 1985-699254	A 19850207 <--
	EP 1986-100544	A 19860117 <--
	GB 1986-18931	A 19860802 <--
	US 1987-78545	A1 19870728 <--
	US 1989-322364	B2 19890313 <--

OTHER SOURCE(S): CASREACT 105:226214  
 ED Entered STN: 26 Dec 1986  
 GI

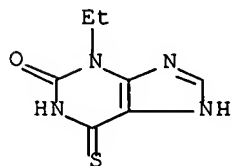


AB The title compds. I (R = Et, Pr, Bu; R1 = H, Me, Et) useful as bronchodilators (no data) were prepared. Thus, 3-ethylxanthine in pyridine was treated with P2S5, H2O, NaOH, and acidified with 5N HCl to give I (R = Et; R1 = H).

IT 105396-64-3P 105396-65-4P 105396-66-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, as bronchodilator)

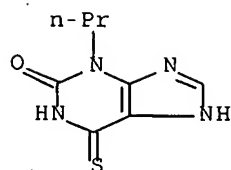
RN 105396-64-3 CAPLUS

CN 2H-Purin-2-one, 3-ethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)

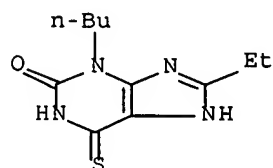


RN 105396-65-4 CAPLUS

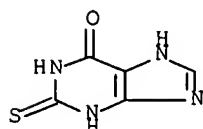
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 105396-66-5 CAPLUS  
 CN 2H-Purin-2-one, 3-butyl-8-ethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)

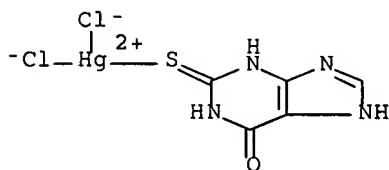


L57 ANSWER 46 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1986:563883 CAPLUS Full-text  
 DOCUMENT NUMBER: 105:163883  
 TITLE: Thermal studies on purine complexes. XI. Thermal behavior of 2-thioxanthine, its chlorohydrate and some thioxanthine complexes of silver(I), cadmium(II), mercury(II) and mercury(I)  
 AUTHOR(S): Sanchez-Sanchez, M. P.; Salas-Peregrin, J. M.; Romero-Molina, M. A.  
 CORPORATE SOURCE: Fac. Sci., Univ. Granada, Granada, 18071, Spain  
 SOURCE: Thermochemica Acta (1986), 102, 149-62  
 CODEN: THACAS; ISSN: 0040-6031  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 01 Nov 1986  
 AB The hydrochloride of 6-oxo-2-thiopurine (LH) was prepared in an acid medium, as well as some Ag(I), Cd(II), Hg(II), and Hg(I) complexes of LH. These compds. were characterized by IR and 1H NMR spectroscopic techniques and thermal anal. (thermogravimetry (TG), differential TG, DSC). Dehalogenation enthalpies were calculated  
 IT 2487-40-3DP, mercury and silver complexes 104626-28-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and thermal decomposition of)  
 RN 2487-40-3 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



RN 104626-28-0 CAPLUS

CN Mercury, dichloro(1,2,3,7-tetrahydro-2-thioxo-6H-purin-6-one-S) - (9CI)  
(CA INDEX NAME)

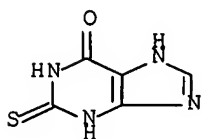


IT 104187-16-8P 104626-27-9P 104626-29-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, heat of dechlorination and thermal decomposition of)

RN 104187-16-8 CAPLUS

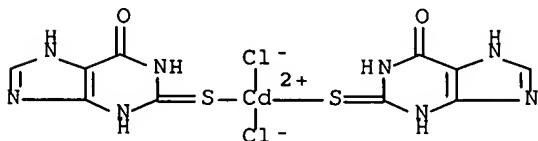
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

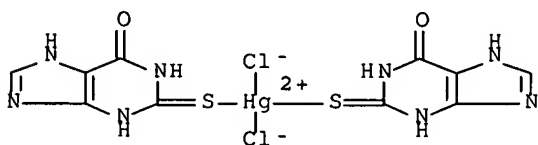
RN 104626-27-9 CAPLUS

CN Cadmium, dichlorobis(1,2,3,7-tetrahydro-2-thioxo-6H-purin-6-one-S) -, (T-4) - (9CI) (CA INDEX NAME)

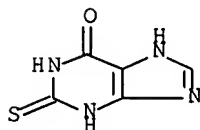


RN 104626-29-1 CAPLUS

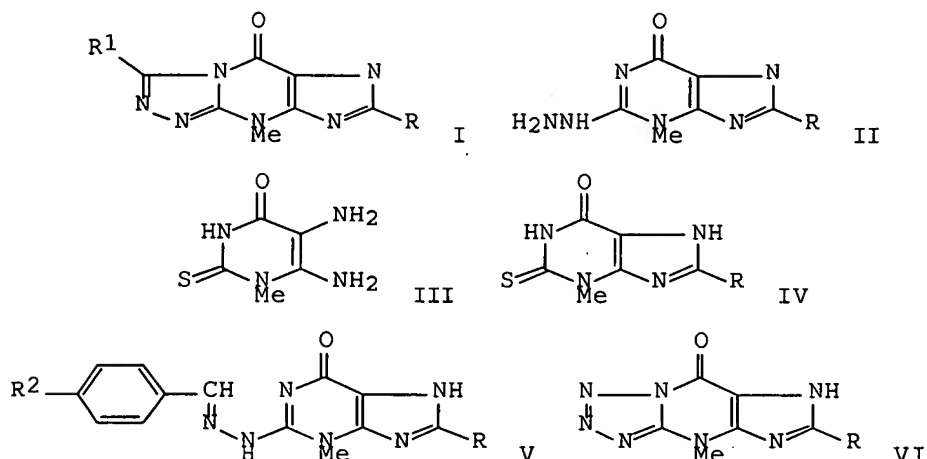
CN Mercury, dichlorobis(1,2,3,7-tetrahydro-2-thioxo-6H-purin-6-one-S) -, (T-4) - (9CI) (CA INDEX NAME)



IT 2487-40-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction with hydrochloric acid, heat of fusion and thermal study of)  
 RN 2487-40-3 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 47 OF 116 CAPLUS · COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1986:478896 CAPLUS Full-text  
 DOCUMENT NUMBER: 105:78896  
 TITLE: Syntheses of 4-methyl-s-triazolo[4,3-a]purin-9(4H)-ones and tetrazolo[1,5-a]purin-9(4H)-ones as aza analogs of "Y" bases  
 AUTHOR(S): Nagamatsu, Tomohisa; Ukai, Masayoshi; Yoneda, Fumio; Brown, Desmond J.  
 CORPORATE SOURCE: Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, 862, Japan  
 SOURCE: Chemical & Pharmaceutical Bulletin (1985), 33(8), 3113-21  
 CODEN: CPBTAL; ISSN: 0009-2363  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 105:78896  
 ED Entered STN: 06 Sep 1986  
 GI



AB 4-Methyl-s-triazolo[4,3-a]purin-9(4H)-ones I (R = H, Me, Et, Ph; R1 = H, Me, Et) were prepared by the cyclocondensation of purin-6(3H)-ones II (R = same) with the appropriate R1C(OEt)3. II were prepared by cyclizing pyrimidine III with RC(OEt)3 and treating the resulting thioxanthines IV with NH2NH2. I [R =



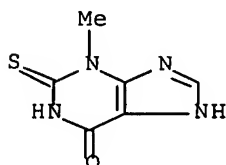
Me, Et, Ph; R1 = p-R2C6H4 (R2 = H, Me, Cl, OMe)] were prepared by the condensation of the appropriate II with p-R2C6H4CHO, followed by the oxidative cyclization of the resulting arylidenehydrazine derivs. V. I (R = Me, Et; R1 = SH, SMe, SEt, SCH2CONH2) were also prepared. Tetrazolo[1,5-a]purin-9(4H)-ones VI (R = H, Me, Et, Ph) were prepared by treating the corresponding II with NaNO2/HCl.

IT 28139-02-8P 91725-06-3P 103289-69-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with hydrazine)

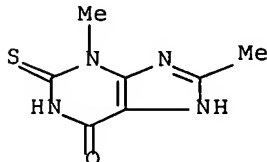
RN 28139-02-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



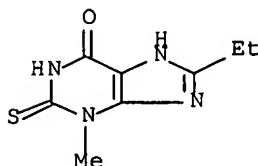
RN 91725-06-3 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3,8-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 103289-69-6 CAPLUS

CN 6H-Purin-6-one, 8-ethyl-1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 48 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

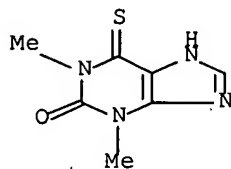
ACCESSION NUMBER: 1986:178050 CAPLUS Full-text

DOCUMENT NUMBER: 104:178050

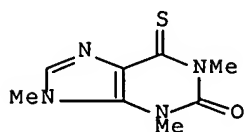
TITLE: 1,3-Dimethyl-2-oxo-6-thioxo-1,2,3,6-tetrahydropurine (S-theophylline)

AUTHOR(S): Benetollo, F.; Bombieri, G.; Dell'Acqua, L.; Fassina,

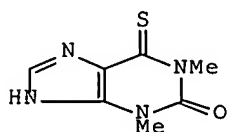
G.  
 CORPORATE SOURCE: Inst. Chem. Technol. Radioelec., CNR, Padua, 35100, Italy  
 SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications (1986), C42(3), 325-7  
 CODEN: ACSCEE; ISSN: 0108-2701  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 17 May 1986  
 AB The title compound is orthorhombic, space group Pbn21, with a 15.614(3), b 8.338(2), and c 6.570(2) Å; dc = 1.52 for Z = 4. Final R = 0.053 for 650 reflections. Atomic coordinates are given. The bond lengths and angles are normal for purine derivs., with the 5- and 6-membered rings and S atom planar. The S-theophylline mols., in contrast to the theophylline ones, are linked in chains by intermol. H bonding (N...O 2.704(9) Å), but do not form the dimers found in the theophylline structure.  
 IT 2398-70-1  
 RL: PRP (Properties)  
 (crystal structure of)  
 RN 2398-70-1 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 49 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1985:571723 CAPLUS Full-text  
 DOCUMENT NUMBER: 103:171723  
 TITLE: A caffeine analog (1,3,7-trimethyl-6-thioxo-2-oxopurine) with a negative inotropic and chronotropic effect  
 AUTHOR(S): Fassina, G.; Gaion, R. M.; Caparrotta, L.; Carpenedo, F.  
 CORPORATE SOURCE: Dep. Pharmacol., Univ. Padova, Padua, I-35131, Italy  
 SOURCE: Naunyn-Schmiedeberg's Archives of Pharmacology (1985), 330(3), 222-6  
 CODEN: NSAPCC; ISSN: 0028-1298  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 30 Nov 1985  
 GI



I



II

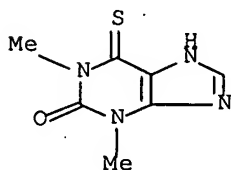
AB Cardiac effects of thioxanthine derivs., 6-thiocaffeine (I) [13182-58-6] and 6-thiotheophylline (II) [2398-70-1], were studied on isolated guinea pig atria and on partially purified cardiac cAMP phosphodiesterase [9036-21-9] enzymes. Theophylline [58-55-9] and caffeine [58-08-2] were used as reference compds. On elec. driven left atria I (0.01-1 mmol/L) decreased contractile tension in a concentration dependent manner. On spontaneously beating atria, the same concns. of I showed neg. inotropic as well as neg. chronotropic effects. On elec. driven left atria, II (0.01-1 mmol/L) increased heart contractile tension but, at higher concns., a reversal of the stimulating effect was observed. Both I and II inhibited bovine heart cAMP phosphodiesterase activity to a comparable extent. Their inhibitory potencies were about 2 and 9-fold higher than those of theophylline or caffeine but consistently lower than that of IBMX. Thus, the replacement of O and S in the methylxanthine mol. drastically modifies the effect induced by the drugs on cardiac function without changing those on cAMP phosphodiesterase.

IT 2398-70-1

RL: BIOL (Biological study)  
(heart rate and contraction response to)

RN 2398-70-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 50 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1984:630460 CAPLUS Full-text

DOCUMENT NUMBER: 101:230460

TITLE: Studies on ring-fused mesoionic thiazolo[3,2-a]imidazolo[4,5-d]pyrimidine derivatives

AUTHOR(S): Talukdar, P. B.; Sengupta, S. K.; Datta, A. K.

CORPORATE SOURCE: Res. Dev. Div., East India Pharm. Works Ltd., Calcutta, 700 061, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1984), 23B(4), 316-20

CODEN: IJSBDB; ISSN: 0376-4699

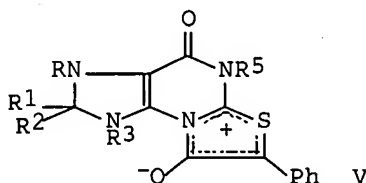
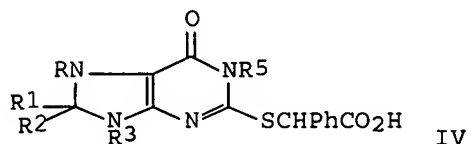
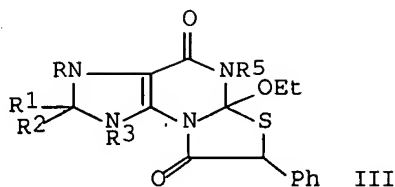
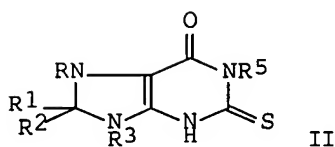
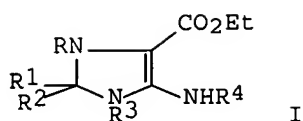
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 101:230460

ED Entered STN: 22 Dec 1984

GI



AB Aminoimidazole esters I (RR1, R1R3 = bond; R = Me; R2 = H, CH2Ph, SMe; R3 = H, Me; R4 = H) were treated with isothiocyanates R5NCS (R5 = Me, Ph) to give thiourea derivs. I [R4 = C(S)NHR5], which cyclized to give oxopurines II. The oxopurines underwent cyclocondensation with ClCHPhCO2Et to give imidazopyrimidine lactams III, which were hydrolyzed to give thiopurines IV. Cyclodehydration of IV (RR1 = bond; R2 = R3 = H; R5 = Me, Ph) gave the N-acylated mesoionic compds. V (R = Ac; R1R3 = bond; R2 = H; R5 = Me, Ph), and thiopurines IV (RR1 = bond, R2 = PhCH2, R3 = H, R5 = Me; R = Me, R1R3 = bond, R2 = CH2Ph, R5 = Me) gave the non-acylated V (R = H) on similar treatment. Treating the mesoionic compds. with EtOH regenerated the imidazopyrimidine lactams.

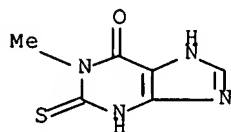
IT 91184-08-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclocondensation of, with chloro(phenyl)acetate, imidazopyrimidine lactam by)

RN 91184-08-6 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1-methyl-2-thioxo- (9CI) (CA INDEX NAME)



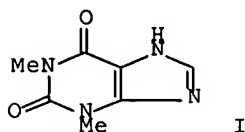
L57 ANSWER 51 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1983:154921 CAPLUS Full-text

DOCUMENT NUMBER: 98:154921

TITLE: New derivatives of methylxanthines: effect of thiocaffeine, thiotheophylline, and 8-phenyltheophylline on lipolysis and on phosphodiesterase activities

AUTHOR(S): Scotini, E.; Carpenedo, F.; Fassina, G.  
 CORPORATE SOURCE: Inst. Pharmacol., Padua Univ., Padua, Italy  
 SOURCE: Pharmacological Research Communications (1983), 15(2), 131-43  
 CODEN: PLRCAT; ISSN: 0031-6989  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 12 May 1984  
 GI



AB The effects of theophylline (I) (TH) [58-55-9], caffeine (CAFF) [58-08-2], 6-thiotheophylline (S-TH) [2398-70-1], 6-thiocaffeine (S-CAFF) [13182-58-6], 8-phenyltheophylline (8-PT) [961-45-5], 3-isobutyl-1-methylxanthine (IBMX) [28822-58-4] on spontaneous and norepinephrine [51-41-2]-induced lipolysis and on cAMP phosphodiesterase (cAMP-PDE) [9036-21-9] activities of rat fat cells were studied. These agents stimulated lipolysis. 8-PT was the most potent compound. Thiocaffeine and thiotheophylline had the least potent activities. IBMX and theophylline had intermediate potencies. The order of potency of the same drugs in potentiating norepinephrine-stimulated lipolysis was: IBMX > 8-PT > S-CAFF > S-TH > CAFF > TH. The rank order of potency to inhibit cAMP-PDE was: IBMX > S-TH and S-CAFF > TH » 8-PT (ineffective). Thus, thiocaffeine and thiotheophylline were more potent than the parent compound theophylline in inhibiting cAMP-PDE, although lipolysis stimulating activities of these compds. were much lower. In contrast, 8-PT stimulated both spontaneous and norepinephrine-induced lipolysis, even though the compound did not inhibit PDE. Some correlation was observed between the order of the antiadenosine activity of these compds. as reported in the literature and their ability to stimulate basal lipolysis. Both antiadenosine and antiPDE activities appear to be involved in modulating hormone-induced lipolysis.

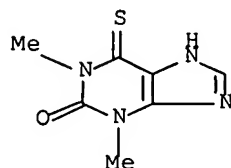
IT 2398-70-1

RL: BIOL (Biological study)

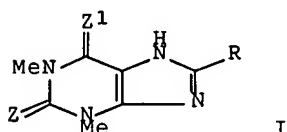
(lipolysis by and PDE activities in adipose tissue response to)

RN 2398-70-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



DOCUMENT NUMBER: 98:125211  
 TITLE: Comparison of the mass spectra of 6-thiotheophyllines and 6-sulfinyltheophyllines  
 AUTHOR(S): Bergmann, Felix; Rahat, Miriam; Frank, Arie; Deutsch, Joseph  
 CORPORATE SOURCE: Dep. Pharmacol., Hebrew Univ.-Hadassah Med. Sch., Jerusalem, Israel  
 SOURCE: Organic Mass Spectrometry (1982), 17(11), 565-8  
 CODEN: ORMSBG; ISSN: 0030-493X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 12 May 1984  
 GI

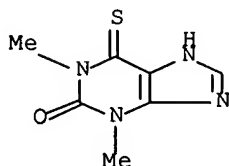


AB Under electron impact, 6-thiotheophyllines (I; Z = O, S; Z1 = S; R = H, Ph) eliminate various fragments from the pyrimidine moiety. In a retro-Diels-Alder reaction, they lose the fragment Z:C:NMe<sub>3</sub> from positions 1 and 2 of the pyrimidine ring. In 6-sulfinyltheophyllines (I; Z = O, S; Z1 = SO; R = H, Ph) the sulfinyl group is the main target for fragmentation; it loses either O or S, and the abundance of [M-16]<sup>+</sup> and [M-32]<sup>+</sup> is much higher than that of the mol. ion. Elimination of the S of the 6-sulfinyl substituent, with retention of its O, is due to formation of a cyclic C-O-S intermediate. All further fragmentations of I (Z1 = SO) proceed via primary O or S loss, followed by elimination of fragments from the pyrimidine moiety, similar to the primary processes observed in the mass spectra of I (Z1 = S).

IT 2398-70-1 6501-94-6 14156-64-0  
 84959-31-9  
 RL: PRP (Properties)  
 (mass spectrum of, fragmentation mechanism in)

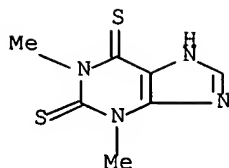
RN 2398-70-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)

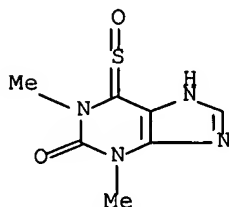


RN 6501-94-6 CAPLUS

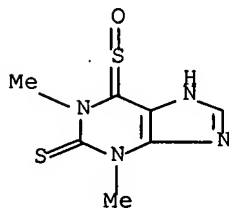
CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



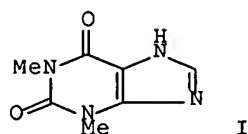
RN 14156-64-0 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-sulfinyl- (9CI) (CA  
 INDEX NAME)



RN 84959-31-9 CAPLUS  
 CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl-, S6-oxide (9CI) (CA  
 INDEX NAME)



L57 ANSWER 53 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1983:119142 CAPLUS Full-text  
 DOCUMENT NUMBER: 98:119142  
 TITLE: Alkylxanthines as adenosine receptor antagonists and  
 membrane phosphodiesterase inhibitors in central  
 nervous tissue: evaluation of structure-activity  
 relationships  
 AUTHOR(S): Wu, P. H.; Phillis, J. W.; Nye, M. J.  
 CORPORATE SOURCE: Coll. Med., Univ. Saskatchewan, Saskatoon, SK, Can.  
 SOURCE: Life Sciences (1982), 31(25), 2857-67  
 CODEN: LIFSAK; ISSN: 0024-3205  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 12 May 1984  
 GI



AB A series of alkylxanthines were examined as antagonists of the adenosine [58-61-7] A<sub>1</sub>-receptor in rat brain synaptosomal membranes and as inhibitors of membrane phosphodiesterase [9025-82-5]. Structure-activity relations showed that the addition of certain substituting groups at position 8 of the theophylline mol. produced mol. structures which generally favored adenosine receptor antagonism. This is evident from the potency order of 8-substituted theophyllines as adenosine receptor antagonists: 8-(p-bromophenyl)theophylline [63325-99-5], 8-(p-methylphenyl)theophylline [57196-70-0], 8-phenyltheophylline [961-45-5] and 8-(p-chlorophenyl)theophylline [29064-02-6], 8-(methoxyphenyl)theophylline [84942-90-5] > 8-(dimethylaminophenyl)theophylline [54013-59-1] > 8-benzyltheophylline [2879-15-4] > theophylline (I) [58-55-9]. The order of potency for inhibition of brain membrane phosphodiesterase was: 1,3-dimethyl-2,6-dithioxopurine [6501-94-6] > methylxanthines > 8-substituted theophyllines. 8-Substituted theophyllines may be selective in their activity as adenosine receptor antagonists, whereas an increase in lipid solubility by substitution at the 1, 2, 3, and 6 positions of the purine ring may result in an increase in phosphodiesterase inhibition.

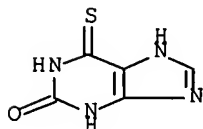
IT 2002-59-7 2398-70-1 2487-40-3  
5437-25-2 6501-94-6 6603-63-0

RL: BIOL (Biological study)

(adenosine receptor and phosphodiesterase of synaptosome membrane response to, alkylxanthines effect on)

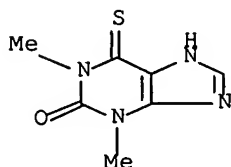
RN 2002-59-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



RN 2398-70-1 CAPLUS

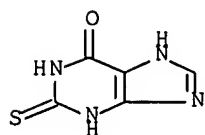
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 2487-40-3 CAPLUS



CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



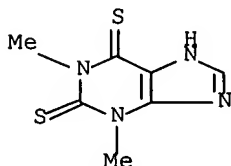
RN 5437-25-2 CAPLUS

CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



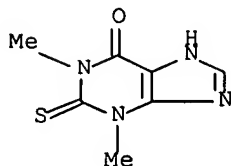
RN 6501-94-6 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



RN 6603-63-0 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 54 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1981:435269 CAPLUS Full-text

DOCUMENT NUMBER: 95:35269

TITLE: Adenosine antagonism by purines, pteridines, and benzopteridines in human fibroblasts

AUTHOR(S): Bruns, Robert F.

CORPORATE SOURCE: Dep. Neurosci., Univ. California, La Jolla, CA, 92093,

USA  
 SOURCE: Biochemical Pharmacology (1981), 30(4),  
 325-33  
 CODEN: BCPCA6; ISSN: 0006-2952  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

ED Entered STN: 12 May 1984

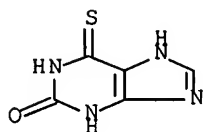
AB Testing of >100 purine bases and structurally related heterocycles as adenosine (I) [58-61-7] antagonists in VA13 fibroblasts (determined by cAMP increase) yielded 3 families of I antagonists: xanthines, benzo[g]pteridines, and 9-substituted adenines. For the xanthines, the optimal group at the 1-position was Bu (5-fold improvement vs. Me), at the 7-position was 2-chloroethyl (5-fold improvement vs. H), and at the 8-position was p-bromophenyl (100-fold improvement vs. H). The receptors apparently had butyl- and phenyl-sized pockets at the 1- and 8-positions, resp., since compds. with larger groups had greatly reduced activity.

IT 2002-59-7 6603-63-0 42458-91-3

RL: BIOL (Biological study)  
 (adenosine receptor of fibroblast antagonism by)

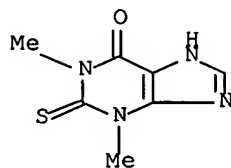
RN 2002-59-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



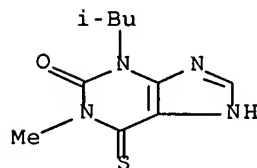
RN 6603-63-0 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 42458-91-3 CAPLUS

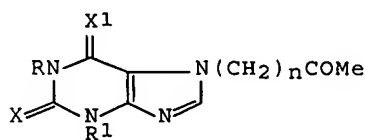
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 55 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1981:139844 CAPLUS Full-text  
 DOCUMENT NUMBER: 94:139844  
 TITLE: Xanthine derivatives and their use in pharmaceutical compositions  
 INVENTOR(S): Goring, Joachim Ewald  
 PATENT ASSIGNEE(S): Wuelfing, Johann A., Fed. Rep. Ger.  
 SOURCE: Eur. Pat. Appl., 30 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 18136	A1	19801029	EP 1980-301053	19800402 <--
EP 18136	B1	19831116		
R: AT, BE, CH, DE, FR, GB, IT, NL, SE				
CA 1128509	A1	19820727	CA 1980-348928	19800401 <--
DK 8001485	A	19801006	DK 1980-1485	19800402 <--
DK 147795	B	19841210		
DK 147795	C	19850819		
ES 490290	A1	19811016	ES 1980-490290	19800402 <--
AU 8057190	A	19810115	AU 1980-57190	19800403 <--
AU 531481	B2	19830825		
ZA 8002010	A	19810429	ZA 1980-2010	19800403 <--
JP 55141487	A	19801105	JP 1980-45090	19800405 <--
US 4454138	A	19840612	US 1982-363125	19820429 <--
PRIORITY APPLN. INFO.:			GB 1979-12052	A 19790405 <--
			GB 1979-19505	A 19790605 <--
			US 1980-135285	A1 19800331 <--

OTHER SOURCE(S): MARPAT 94:139844  
 ED Entered STN: 12 May 1984  
 GI

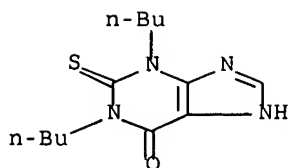


AB Thioxanthine I (X, X1 = O, S; n = 1, 2; R, R1 = alkyl) were prepared Thus, 4 g 1-butyl-3-ethyl-6-thioxanthine was treated with 2.7 g BrCH2COMe to give 1 g I (R = Bu, R1 = Et, X = O, X1 = S, n = 2; II). At 2 mg/kg orally II caused a 22.2% increase in the contractility of skeletal muscle in cats.

IT 77038-96-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction of, with bromopropanone)

RN 77038-96-1 CAPLUS

CN 6H-Purin-6-one, 1,3-dibutyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)

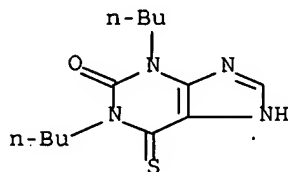


IT 77038-98-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with chloropropanone)

RN 77038-98-3 CAPLUS

CN 2H-Purin-2-one, 1,3-dibutyl-1,3,6,7-tetrahydro-6-thioxo-, sodium salt (9CI) (CA INDEX NAME)



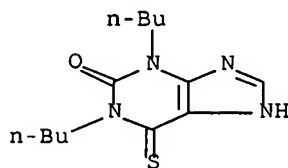
● Na

IT 40915-18-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with Me vinyl ketone)

RN 40915-18-2 CAPLUS

CN 2H-Purin-2-one, 1,3-dibutyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)

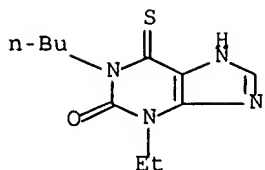


IT 77038-90-5

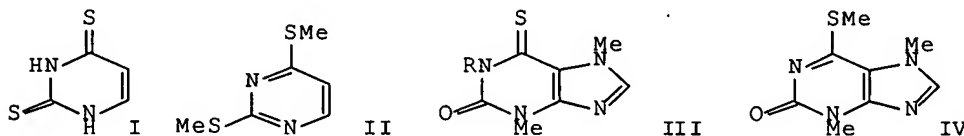
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with bromopropanone)

RN 77038-90-5 CAPLUS

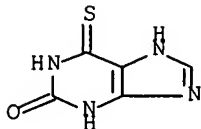
CN 2H-Purin-2-one, 1-butyl-3-ethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



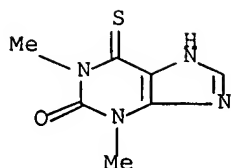
L57 ANSWER 56 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1981:84065 CAPLUS Full-text  
 DOCUMENT NUMBER: 94:84065  
 TITLE: Methylation of thiouracils and thioxanthines with trimethyl phosphate  
 AUTHOR(S): Hayashi, Masahiro; Hisanaga, Yorisato; Yamauchi, Kiyoshi; Kinoshita, Masayoshi  
 CORPORATE SOURCE: Dep. Appl. Chem., Osaka City Univ., Osaka, 558, Japan  
 SOURCE: Synthetic Communications (1980), 10(10), 791-8  
 CODEN: SYNCAV; ISSN: 0039-7911  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 12 May 1984  
 GI



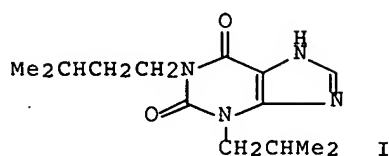
AB Thiouracils and thioxanthines were methylated with (MeO)<sub>3</sub>PO in DMF at 80-100° to give S-methylated derivs. Thus, I gave 85% II. III (R = H) in the presence of Et<sub>3</sub>N gave 51% III (R = Me) and 35% IV.  
 IT 2002-59-7 2398-70-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (methylation of)  
 RN 2002-59-7 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



RN 2398-70-1 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 57 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1980:51769 CAPLUS Full-text  
 DOCUMENT NUMBER: 92:51769  
 TITLE: Effects of phosphodiesterase inhibitors on cyclic nucleotide levels and relaxation of pig coronary arteries  
 AUTHOR(S): Kramer, G. L.; Wells, J. N.  
 CORPORATE SOURCE: Sch. Med., Vanderbilt Univ., Nashville, TN, 37232, USA  
 SOURCE: Molecular Pharmacology (1979), 16(3), 813-22  
 CODEN: MOPMA3; ISSN: 0026-895X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 12 May 1984  
 GI



AB A series of xanthine derivs. and papaverine were studied to determine their abilities to alter tissue levels of cyclic AMP [60-92-4] and cyclic GMP [7665-99-8], inhibit cyclic nucleotide phosphodiesterase [50812-31-2] activities, and cause relaxation of pig coronary arteries. The agents exhibited a wide range of potencies to inhibit phosphodiesterase activities in the coronary artery supernatant fraction. In addition, some of these agents were up to 10 times more potent as inhibitors of cyclic GMP hydrolysis than of cyclic AMP hydrolysis, whereas others were 2-4 times more potent as inhibitors of cyclic AMP than of cyclic GMP hydrolysis. The rank order of potencies of these agents to cause relaxation of coronary artery strips was similar to the rank order of potencies to inhibit cyclic nucleotide phosphodiesterase activities. There were, however, some notable exceptions to the correlation between inhibition of cyclic nucleotide phosphodiesterase activities and relaxation. 1-Isoamyl-3-isobutylxanthine (I) [63908-26-9] was a more potent relaxing agent than might be expected from its relatively low potency to inhibit cyclic nucleotide hydrolysis in tissue exts. On the other hand, 1-methyl-3-isobutyl-7-(3-chlorobenzyl)-xanthine [58481-28-0] was 1 of the more potent inhibitors of cyclic nucleotide hydrolysis but was not as potent in causing relaxation as might have been expected. Exposure of the coronary artery strips to inhibitors caused increase in tissue levels of cyclic AMP and cyclic GMP and there was a statistically significant multiple linear regression of cyclic AMP and cyclic GMP levels on percent relaxation after 5

min of exposure to the agents. Cyclic AMP and cyclic GMP levels made approx. equal contributions to the regression of changes in percent relaxation, as determined by anal. of variance methods. While I did not fit the correlation between phosphodiesterase inhibition and potency to relax the arterial strips as well as the other agents, this agent caused unexpectedly large increases in cyclic AMP levels. Some agents caused relaxation accompanied by significant elevation of cyclic GMP levels and no significant change in cyclic AMP levels while other agents caused relaxation accompanied by significant increases in cyclic AMP but not cyclic GMP. These data offer some support for a hypothesis that both cyclic AMP and cyclic GMP are involved in the relaxation processes of pig coronary arteries.

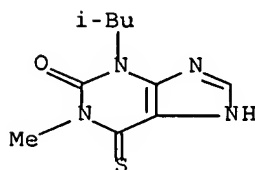
IT 42458-91-3

RL: BIOL (Biological study)

(cyclic nucleotide of artery and artery contraction response to)

RN 42458-91-3 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 58 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1979:570643 CAPLUS Full-text

DOCUMENT NUMBER: 91:170643

TITLE: Behavior of N-methylated allopurinols and related 4-thioxopyrazolo[3,4-d]pyrimidines towards bovine milk xanthine oxidase

AUTHOR(S): Bergmann, Felix; Frank, Arie; Govrin, Hanna

CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel

SOURCE: Biochimica et Biophysica Acta, Enzymology (

1979), 570(1), 215-20

CODEN: BBEZAD; ISSN: 0924-1086

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 12 May 1984

AB All available N-mono- and N,N'-dimethylallopurinols and the corresponding 4-thioxo derivs. were tested as substrates or inhibitors of bovine milk xanthine oxidase (EC 1.2.3.2). None of the compds. tested revealed any inhibitory activity towards the enzyme. All compds. were resistant to enzymic oxidation, with the exception of 7-methylallopurinol and its 4-thioxo analog. Both these compds. were attacked at position 6. 7-Methylallopurinol was oxidized nearly 10-fold faster than the isomeric 3-methylhypoxanthine. These observations can be explained by assuming that for attack at C-6, the enzyme must bind both to N-1 and N-2 in the pyrazole ring and causes tautomerization, which places a double bond at position 5,6 in the pyrimidine ring. This activation process resembles the activation of hypoxanthine.

IT 33285-76-6

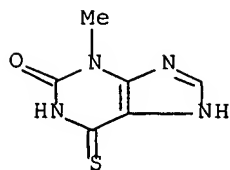
RL: BIOL (Biological study)

(xanthine oxidase response to)

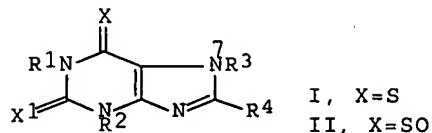
RN 33285-76-6 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX

NAME)



L57 ANSWER 59 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1977:453218 CAPLUS Full-text  
 DOCUMENT NUMBER: 87:53218  
 TITLE: 6-Sulfinyl derivatives of xanthines  
 AUTHOR(S): Bergmann, Felix; Frank, Arie; Weiler-Feilchenfeld, Hanna; Tamir, Ilana  
 CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel  
 SOURCE: Journal of Organic Chemistry (1977), 42(14), 2470-3  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 12 May 1984  
 GI



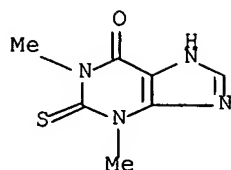
AB 6-Thiopurines I (R1 = R4 = H, R2 = R3 = Me, X1 = O; R1 = R2 = Me, R3 = R4 = H, X1 = O, S; R1 = R2 = Me, R3 = H, R4 = Ph, X1 = O, S) are oxidized by H2O2 or by BzOOH to 6-sulfinylpurines II. Only theophylline derivs. of these unstable II were obtained in pure form. The isomers formed have the 6-sulfinyl group directed toward the 7-NH due to stabilization by an intramol. H bridge. Their structure has been derived from dipole moments and from the chemical shift of the 1-Me substituent. The 2-thiocarbonyl group in 2-thiotheophyllines is not attacked by the oxidants used, which convert 6-selenoxanthines to the corresponding xanthines.

IT 6603-63-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclization of)

RN 6603-63-0 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



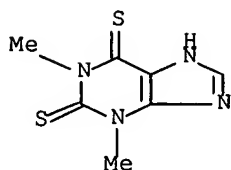


IT 6501-94-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and oxidation of)

RN 6501-94-6 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)

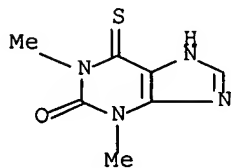


IT 2398-70-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and reactions of)

RN 2398-70-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)

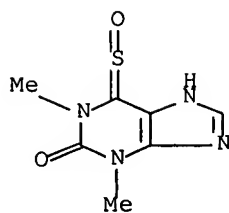


IT 62006-25-1P 62006-26-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

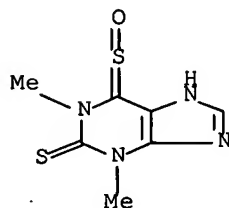
RN 62006-25-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-sulfinyl-, (E)- (9CI)  
(CA INDEX NAME)



RN 62006-26-2 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl-, S6-oxide, (E)- (9CI)  
(CA INDEX NAME)



L57 ANSWER 60 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1977:133356 CAPLUS Full-text

DOCUMENT NUMBER: 86:133356

TITLE: Effects of adenosine and related compounds on  
adenylate cyclase and cyclic AMP levels in smooth  
muscle

AUTHOR(S): McKenzie, Sheila G.; Frew, Robert; Bar, Hans P.

CORPORATE SOURCE: Dep. Pharmacol., Univ. Alberta, Edmonton, AB, Can.

SOURCE: European Journal of Pharmacology (1977),  
41(2), 193-203

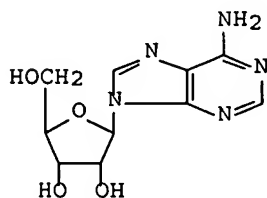
CODEN: EJPHAZ; ISSN: 0014-2999

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 12 May 1984

GI



I

AB The hypotheses were tested that the relaxant effect of adenosine (I) [58-61-7] and related compds. in the longitudinal muscle of the rabbit small intestine involves interaction with adenylylase [9012-42-4] and/or the elevation of tissue cyclic AMP [60-92-4] levels. Adenylylase was prepared by

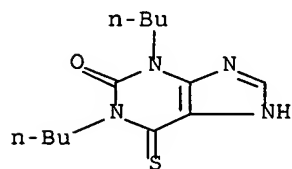
gentle homogenization of an isolated smooth muscle cell fraction obtained after collagenase digestion of longitudinal muscle strips. A number of analogs and derivs. of I possessing a primary or secondary 6-amino group inhibited the enzyme similarly to I; however, there was no correlation between compds. known to relax the intact tissue and the existence, or the degree of, cyclase inhibition. Isolated muscle strips were exposed to adrenaline bitartrate [51-42-3], DL-isoprenaline-HCl [949-36-0], I, or ATP [56-65-5], at doses causing 30-60% relaxation, for 60 s prior to sampling and anal. of cAMP content. While small increments in cAMP levels were found after administering adrenaline or isoprenaline, no change was found with I in the absence or presence of aminophylline [317-34-0] or 1-methyl-3-isobutylxanthine [28822-58-4]. Neither adenylate cyclase inhibition nor changes in cAMP levels appear to be part of the mechanism of the smooth muscle relaxant action of I or ATP.

IT 40915-18-2 42458-88-8 42458-91-3  
 42458-94-6 42458-97-9 42458-98-0  
 42458-99-1 42459-01-8 42459-06-3  
 42459-07-4

RL: BIOL (Biological study)  
 (adenylate cyclase of intestine smooth muscle response to)

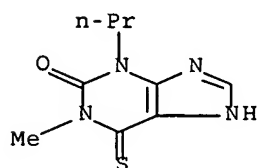
RN 40915-18-2 CAPLUS

CN 2H-Purin-2-one, 1,3-dibutyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



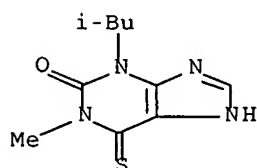
RN 42458-88-8 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)

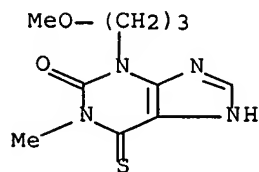


RN 42458-91-3 CAPLUS

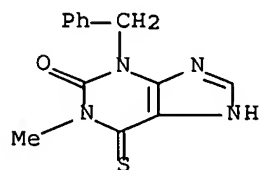
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



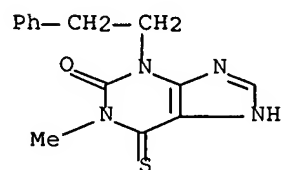
RN 42458-94-6 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(3-methoxypropyl)-1-methyl-6-thioxo-  
(9CI) (CA INDEX NAME)

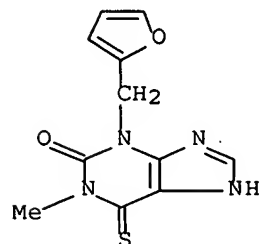
RN 42458-97-9 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(phenylmethyl)-6-thioxo-  
(9CI) (CA INDEX NAME)

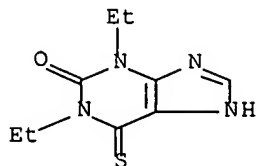
RN 42458-98-0 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-phenylethyl)-6-thioxo-  
(9CI) (CA INDEX NAME)

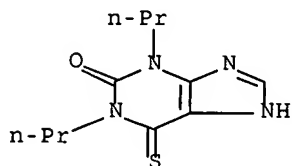
RN 42458-99-1 CAPLUS

CN 2H-Purin-2-one, 3-(2-furanylmethyl)-1,3,6,7-tetrahydro-1-methyl-6-thioxo-  
(9CI) (CA INDEX NAME)

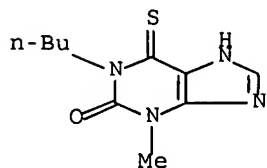
RN 42459-01-8 CAPLUS  
 CN 2H-Purin-2-one, 1,3-diethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



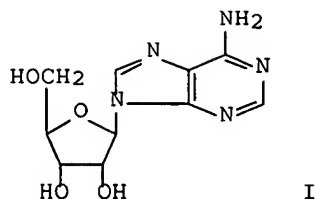
RN 42459-06-3 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dipropyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 42459-07-4 CAPLUS  
 CN 2H-Purin-2-one, 1-butyl-1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 61 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1977:133355 CAPLUS Full-text  
 DOCUMENT NUMBER: 86:133355  
 TITLE: Characteristics of the relaxant response of adenosine and its analogs in intestinal smooth muscle.  
 AUTHOR(S): McKenzie, Sheila G.; Frew, Robert; Bar, Hans P.  
 CORPORATE SOURCE: Dep. Pharmacol., Univ. Alberta, Edmonton, AB, Can.  
 SOURCE: European Journal of Pharmacology (1977), 41(2), 183-92  
 CODEN: EJPHAZ; ISSN: 0014-2999.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 12 May 1984  
 GI



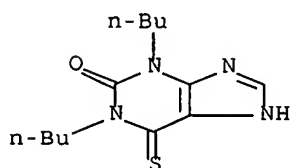
AB Several characteristics of the relaxant response of the isolated longitudinal muscle of the rabbit small intestine in response to the administration of adenosine (I) [58-61-7] and related compds. are studied. Following administration of I or ATP [56-65-5] the preparation responded with a rapid initial suspension of spontaneous contractile activity followed by a secondary sustained phase of inhibition of lower magnitude. Cumulative application of relaxant doses of I or ATP caused a lesser total response than that obtained by single application of the cumulative dose. Neither procaine, lidocaine or guanethidine antagonized the responses to I or ATP and the responsiveness of muscles obtained from reserpinized animals appeared unchanged. A number of I derivs. and analogs was tested for the ability to relax the muscle. Generally, compds. containing a primary or secondary 6-amino group acted as agonists with the exception of 8-bromoadenosine [2946-39-6]. Inactive nucleosides did not modify the responsiveness of the muscle to I. Responses to I and ATP were not appreciably modified by papaverine, imidazole, dipyridamole, 6-(p-nitrobenzylthio)-purine riboside. Antagonism was observed, however, with phentolamine [50-60-2] and aminophylline [317-34-0]. Aminophylline at 100  $\mu$ M inhibited responses to I over a wide dose range; this antagonism was surmountable by high doses of I. 1-Methyl-3-isobutylxanthine [28822-58-4] did not antagonize I responses. A number of 1,3-alkyl-6-thioxanthines did not modify the I response at doses that did not show any direct action. The results support the concept of an extracellular receptor site of I and its analogs and the absence of an indirect mechanism of action via nerve stimulation.

IT 40915-18-2 42458-88-8 42458-91-3  
 42458-94-6 42458-97-9 42458-98-0  
 42458-99-1 42459-01-8 42459-06-3  
 42459-07-4

RL: BIOL (Biological study)  
 (intestine smooth muscle relaxation by adenosine and its analogs  
 response to)

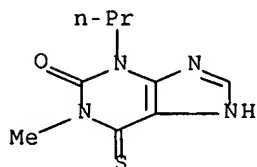
RN 40915-18-2 CAPLUS

CN 2H-Purin-2-one, 1,3-dibutyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX  
 NAME)



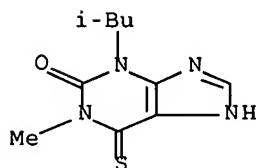
RN 42458-88-8 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



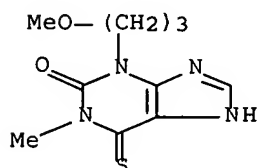
RN 42458-91-3 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



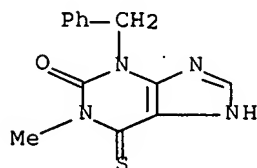
RN 42458-94-6 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(3-methoxypropyl)-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



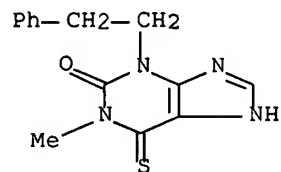
RN 42458-97-9 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(phenylmethyl)-6-thioxo- (9CI) (CA INDEX NAME)



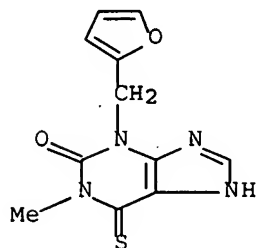
RN 42458-98-0 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-phenylethyl)-6-thio-  
(9CI) (CA INDEX NAME)



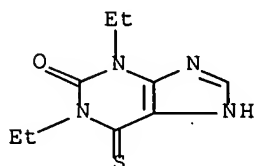
RN 42458-99-1 CAPLUS

CN 2H-Purin-2-one, 3-(2-furanylmethyl)-1,3,6,7-tetrahydro-1-methyl-6-thio-  
(9CI) (CA INDEX NAME)



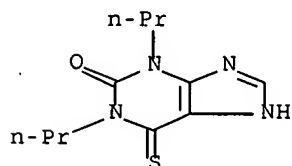
RN 42459-01-8 CAPLUS

CN 2H-Purin-2-one, 1,3-diethyl-1,3,6,7-tetrahydro-6-thio- (9CI) (CA INDEX  
NAME)



RN 42459-06-3 CAPLUS

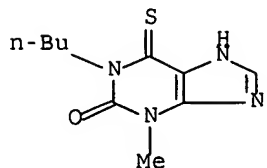
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dipropyl-6-thio- (9CI) (CA INDEX  
NAME)



RN 42459-07-4 CAPLUS



CN 2H-Purin-2-one, 1-butyl-1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 62 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1976:561303 CAPLUS Full-text  
 DOCUMENT NUMBER: 85:161303  
 TITLE: Heat stabilizers for vinyl halide resins  
 INVENTOR(S): Sekiguchi, Tetsuo; Abe, Masami; Tsuruga, Koji;  
 Tominaga, Nobuhide  
 PATENT ASSIGNEE(S): Adeka Argus Chemical Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 51088542	A	19760803	JP 1975-13797	19750131 <--
PRIORITY APPLN. INFO.:			JP 1975-13797	A 19750131 <--

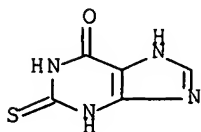
ED Entered STN: 12 May 1984

AB PVC [9002-86-2] (optionally containing ABS [9003-56-9]) and poly(vinyl fluoride) [24981-14-4] contained heterocyclic compds. containing -N:C(SH)NRC(:R1)- groups (R = H, alkyl, aryl; R1 = O, S; including tautomeric forms or salts) as heat stabilizers. For example, a PVC composition containing DOP 50, epoxidized soybean oil 2, tris(nonylphenyl) phosphite 0.5, stearic acid 0.5, and 3,5-dimercapto-1,2,4-triazole (I) [5650-03-3] 0.05 phr had heat stability (175°) 60 min, compared with 30 min for a control not containing I.

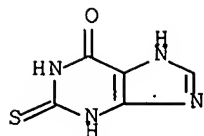
IT 2487-40-3 60682-54-4  
 RL: MOA (Modifier or additive use); USES (Uses)  
 (heat stabilizers, for vinyl halide resins)

RN 2487-40-3 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



RN 60682-54-4 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo-, barium salt (1:1) (9CI) (CA INDEX NAME)



● Ba

L57 ANSWER 63 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1976:470075 CAPLUS Full-text  
 DOCUMENT NUMBER: 85:70075  
 TITLE: Copper electroplating from pyrophosphate baths  
 INVENTOR(S): Nakamura, Minoru; Minagawa, Tadashi; Asai, Osamu  
 PATENT ASSIGNEE(S): Hitachi, Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 51021529	A	19760220	JP 1974-93391	19740816 <--
PRIORITY APPLN. INFO.:			JP 1974-93391	A 19740816 <--

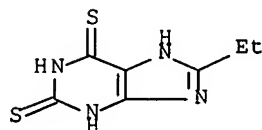
ED Entered STN: 12 May 1984

AB The formation of brittle films on Cu electroplates produced in a Cu<sub>2</sub>P<sub>2</sub>O<sub>7</sub> bath is prevented by adding, prior to or following embrittlement, an embrittlement inhibitor 0.00001-0.1 g/l. to a plating bath with a H<sub>4</sub>P<sub>2</sub>O<sub>7</sub>/Cu ratio of 9.2-8.5. The embrittlement inhibitor was ≥1 compds. selected from mercaptopurines, mercaptopyrazineimidazoles, mercaptopyrazinethiazoles, mercaptopyridinethiazoles and their alkyl, amino, Ph, or OH derivs. Thus, Cu was plated on stainless steel in a bath containing Cu<sub>2</sub>P<sub>2</sub>O<sub>7</sub>·3H<sub>2</sub>O 70, K<sub>4</sub>P<sub>2</sub>O<sub>7</sub> 316 g/l., 27% NH<sub>4</sub>OH 5 ml/l., KNO<sub>3</sub> 15 g/l. and 2,6-dimercapto-8-ethylpurine (I) 1 mg/l. at a pH of 8.5, a bath temperature of 55°, an anode c.d. of 4.5 A/dm<sup>2</sup>, a cathode c.d. of 3.0 A/dm<sup>2</sup>, and air stirring. The formation of a brittle film did not occur up to 45-55 hr. In contrast, embrittlement occurred within 20-25 hr in the absence of I.

IT 60022-13-1  
 RL: PRP (Properties)  
 (in electroplating, embrittlement inhibitor for copper)

RN 60022-13-1 CAPLUS

CN 1H-Purine-2,6-dithione, 8-ethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



L57 ANSWER 64 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:416151 CAPLUS Full-text

DOCUMENT NUMBER: 85:16151

TITLE: Oxidation of N-methyl substituted hypoxanthines, xanthines, purine-6,8-diones and the corresponding 6-thioxo derivatives by bovine milk xanthine oxidase

AUTHOR(S): Bergmann, Felix; Levene, Lawrence

CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel

SOURCE: Biochimica et Biophysica Acta, Enzymology (1976), 429(3), 672-88

CODEN: BBEZAD; ISSN: 0924-1086

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 12 May 1984

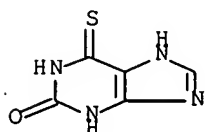
AB The oxidation of 6 series of purines (hypoxanthines, xanthines, purine-6,8-diones, and the corresponding 6-thioxo derivs.) by a highly purified bovine milk xanthine oxidase was studied, using a variety of N-Me derivs. N-Me substituents can either enhance or reduce enzymic rates. Enhancement is ascribed to blockage of groups which mediate unfavorable modes of binding of substrate to enzyme. Introduction of N-Me groups can also inhibit enzymic oxidation, either by occluding essential binding groups or by preventing spontaneous or enzyme-induced tautomerization processes, which create suitable binding sites in the substrates. In all purines which are rapidly attacked by xanthine oxidase, proper attachment to the active center is mediated by the groupings (3)NH, (9)N, or (3)N, (9)NH. Reduced rates usually express lowered substrate affinity, which finds its expression in weak competitive inhibition of xanthine oxidation

IT 2002-59-7 33285-76-6 38695-85-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidation of, enzymic)

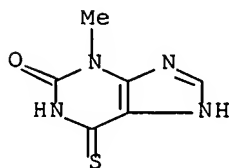
RN 2002-59-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



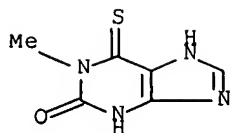
RN 33285-76-6 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)

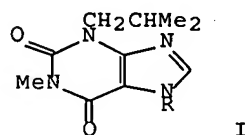


RN 38695-85-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



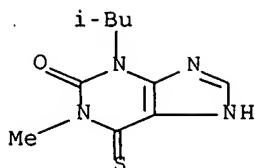
L57 ANSWER 65 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1976:130133 CAPLUS Full-text  
 DOCUMENT NUMBER: 84:130133  
 TITLE: Inhibition of separated forms of phosphodiesterases from pig coronary arteries by uracils and by 7-substituted derivatives of 1-methyl-3-isobutylxanthine  
 AUTHOR(S): Garst, J. E.; Kramer, G. L.; Wu, Y. J.; Wells, J. N.  
 CORPORATE SOURCE: Sch. Med., Vanderbilt Univ., Nashville, TN, USA  
 SOURCE: Journal of Medicinal Chemistry (1976), 19(4), 499-503  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 12 May 1984  
 GI



AB A series of 15 title xanthine derivs. (I; R = alkyl, aralkyl, alicyclicalkyl, propargyl, 4-picolyl), prepared by alkylation of 1-methyl-3-isobutylxanthine (I, R = H) (MIX) [28822-58-4] were tested for specificity of inhibition of chromatog.-separated cyclic nucleotide phosphodiesterase [50812-31-2] activity fractions I and II. I were generally much less potent than MIX as inhibitors of activity fraction II, but some retained the potency of MIX as inhibitors of activity fraction I. 1-Methyl-3-isobutyl-7-benzylxanthine (I, R = PhCH<sub>2</sub>) [58481-23-5] was 20-30 times more potent as an inhibitor of activity fraction I than of II, while retaining the potency of MIX against activity fraction I. A series of 1,3-dialkyluracils had low potency as phosphodiesterase inhibitors. Structure-activity relations were discussed.

IT 42458-91-3  
 RL: BIOL (Biological study)  
 (cyclic nucleotide phosphodiesterases inhibition by)

RN 42458-91-3 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo-(9CI) (CA INDEX NAME)



L57 ANSWER 66 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:105543 CAPLUS Full-text

DOCUMENT NUMBER: 84:105543

TITLE: Thermal decomposition of quaternary hypoxanthinium salts and related purines

AUTHOR(S): Bergmann, Felix; Rahat, Miriam

CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1976), (2), 239-43

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 12 May 1984

GI For diagram(s), see printed CA Issue.

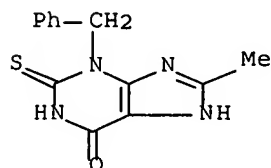
AB Addnl. data considered in abstracting and indexing are available from a source cited in the original document. Thermal decomposition of quaternary hypoxanthinium salts was achieved by heating their solns. in DMF. 1,3-Dialkylhypoxanthinium bromides or iodides lost the 3-substituent as alkyl halide, which then attacked the imidazole ring at N-7 or N-9. Thermolysis of the dioxotetrahydropurinium iodide I (R = H) involved either loss of the 3-Me group as MeI giving the dihydromethylpurinedione II (R = H), or removal of HI to give the corresponding betaine which was then methylated at N-9 to give the dioxotetrahydropurinium iodide I (R = Me). The latter compound in turn decomposed to give the dimethylpurinedione II (R = Me). Similarly, the dimethylhypoxanthinium iodide III (R = H) was degraded mainly by loss of MeI, giving IV (R = H) and small amts. of V (R = H). III (R = H) also lost HI to give the corresponding betaine, which methylated at N-1 to give III (R = Me). III (R = Me) again underwent thermolysis to give a mixture of IV (R = Me) and its 9-Me isomer.

IT 59311-65-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation, reduction, and NMR of)

RN 59311-65-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-8-methyl-3-(phenylmethyl)-2-thioxo-(9CI) (CA INDEX NAME)



L57 ANSWER 67 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:90117 CAPLUS Full-text  
 DOCUMENT NUMBER: 84:90117  
 TITLE: Reactions of 2-, 6-, and 8-monosubstituted 1- and 3-methylpurines with hydroxide ions in water  
 AUTHOR(S): Badger, Rodney J.; Barlin, Gordon B.  
 CORPORATE SOURCE: John Curtin Sch. Med. Res., Aust. Natl. Univ., Canberra, Australia  
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1976), (2), 151-5  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 84:90117

ED Entered STN: 12 May 1984

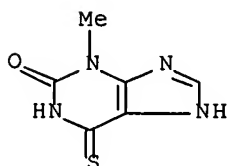
AB 1-Methyl-2- and 6-methylthiopurine underwent nucleophilic displacement with NaOH to give the 2- and 6-hydroxypurine analogs, resp. whereas 1-methyl-8-methylthiopurine underwent ring cleavage to give 5-amino-2-methylthioimidazole-4-carboxaldehyde. 3-Methyl-6-methylthiopurine with NaOH gave predominantly 5-methylaminoimidazole-4-carboxaldehyde, whereas 3-methyl-8-methylthiopurine underwent ring cleavage like its 1-methyl isomer. 7- And 9-methyl-2-methylthiopurines gave 4-amino-5-methylamino- and 5-amino-4-methylamino-2-methylthiopyrimidines, resp. Hydrolysis of 6-chloro-3-methylpurine gave 5-methylaminoimidazole-4-carbonitrile and some 6-hydroxy-3-methylpurine. 8-Chloro-3-methylpurine was hydrolyzed without formation of the 8-hydroxy compound

IT 33285-76-6

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (hydrogenation of)

RN 33285-76-6 CAPLUS

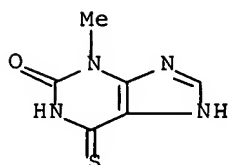
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



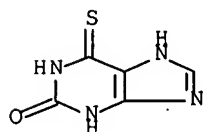
L57 ANSWER 68 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1975:125358 CAPLUS Full-text  
 DOCUMENT NUMBER: 82:125358  
 TITLE: Preparation of some N-methylisoguanines via 6-methylthio-2-oxopurines, and 8-methylisoguanine  
 AUTHOR(S): Kazimierczuk, Z.; Shugar, D.  
 CORPORATE SOURCE: Inst. Exp. Phys., Univ. Warsaw, Warsaw, Pol.  
 SOURCE: Acta Biochimica Polonica (1974), 21(4), 455-63  
 CODEN: ABPLAF; ISSN: 0001-527X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 82:125358  
 ED Entered STN: 12 May 1984

GI For diagram(s), see printed CA Issue.  
 AB Isoguanines I (R-R3 = H, Me) were obtained by reaction of R2R3NH with 6-methylthio-2-oxopurines, prepared by treating the xanthenes with P2S5 and methylating. 8-Methylisoguanine was prepared from 4,5,6-triaminopyrimidin-2-one and AcNH2. The pK values of I and II are reported. II (R = Me, R2 = R3 = H) was resistant to HNO2 deamination, whereas I (R2 = R3 = H) were easily deaminated.  
 IT 33285-76-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 33285-76-6 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)

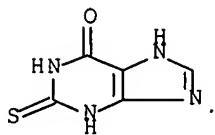


L57 ANSWER 69 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1974:107452 CAPLUS Full-text  
 DOCUMENT NUMBER: 80:107452  
 TITLE: Mass spectra of N- and S-methylpurines  
 AUTHOR(S): Deutsch, J.; Neiman, Z.; Bergmann, F.  
 CORPORATE SOURCE: Dep. Pharm. Chem., Hebrew Univ., Jerusalem, Israel  
 SOURCE: Jerusalem Symposia on Quantum Chemistry and  
 Biochemistry (1972), 4, 402-11  
 CODEN: JSQCA7; ISSN: 0075-3696  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 12 May 1984  
 AB The mass spectra of hypoxanthines, 6-purinethiones, adenines, and 6-(methylamino)purines are given. The 7-Me derivs. of these compds. lose a H atom to give M-1 cation which is stabilized by cyclization. The analogous process occurs in 6-(methylthio)purines by loss of a H atom from the MeS group. The cyclization process is reflected by abundant metastable peaks.  
 IT 2002-59-7 2487-40-3 5437-25-2  
 33285-76-6  
 RL: PRP (Properties)  
 (mass spectrum of)  
 RN 2002-59-7 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



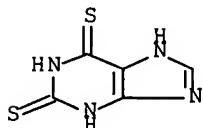
RN 2487-40-3 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



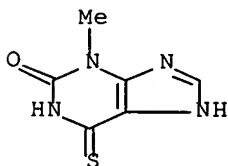
RN 5437-25-2 CAPLUS

CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



RN 33285-76-6 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 70 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1973:427084 CAPLUS Full-text

DOCUMENT NUMBER: 79:27084

TITLE: Structure-activity relations. III. Bronchodilator activity of substituted 6-thioxanthines

AUTHOR(S): Bowden, Keith; Wooldridge, Kenneth R. H.

CORPORATE SOURCE: Dep. Chem., Univ. Essex, Colchester/Essex, UK

SOURCE: Biochemical Pharmacology (1973), 22(9), 1015-21

CODEN: BCPCA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 12 May 1984

AB A correlation of the bronchodilator activity of a series of substituted 6-thioxanthines (I) was made with partition parameters and (or) the steric effect of the 1- and 3-substituents. An increase in activity was observed on introduction of bulky substituents at R3 and particularly at R1. The 3-substituted series were also correlated by a Hansch relation involving partition factors alone. Thus, 1,3-dibutyl-6-thioxanthine [ 40915-18-2] was far more active than 1,3-dimethyl-6-thioxanthine [ 2398-70-1].

IT 2398-70-1 40915-18-2 42458-87-7

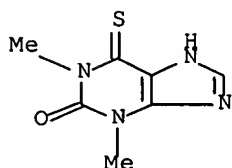


42458-88-8 42458-89-9 42458-90-2  
 42458-91-3 42458-92-4 42458-93-5  
 42458-94-6 42458-95-7 42458-96-8  
 42458-97-9 42458-98-0 42458-99-1  
 42459-00-7 42459-01-8 42459-02-9  
 42459-03-0 42459-04-1 42459-06-3  
 42459-07-4 42459-09-6 42459-10-9

RL: BIOL (Biological study)  
 (bronchodilator)

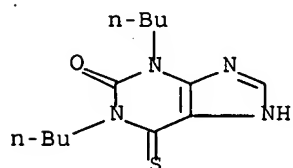
RN 2398-70-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



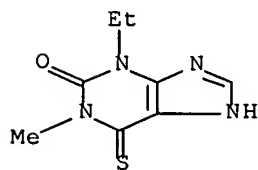
RN 40915-18-2 CAPLUS

CN 2H-Purin-2-one, 1,3-dibutyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



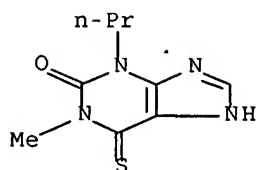
RN 42458-87-7 CAPLUS

CN 2H-Purin-2-one, 3-ethyl-1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



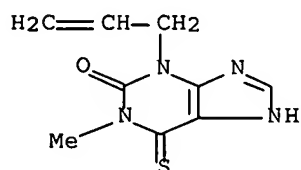
RN 42458-88-8 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



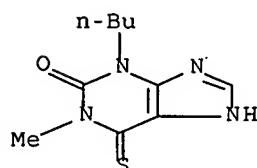
RN 42458-89-9 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-propenyl)-6-thioxo- (9CI)  
(CA INDEX NAME)



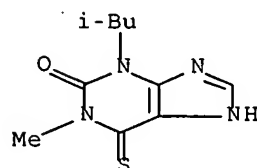
RN 42458-90-2 CAPLUS

CN 2H-Purin-2-one, 3-butyl-1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA  
INDEX NAME)



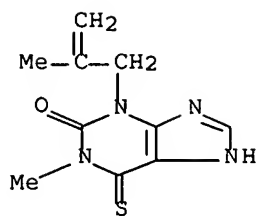
RN 42458-91-3 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo-  
(9CI) (CA INDEX NAME)



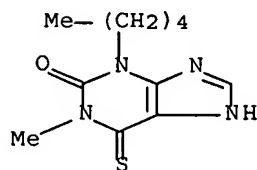
RN 42458-92-4 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methyl-2-propenyl)-6-  
thioxo- (9CI) (CA INDEX NAME)



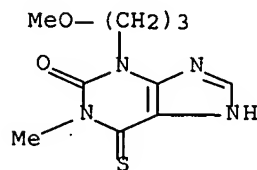
RN 42458-93-5 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-pentyl-6-thioxo- (9CI) (CA INDEX NAME)



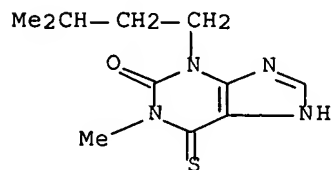
RN 42458-94-6 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(3-methoxypropyl)-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



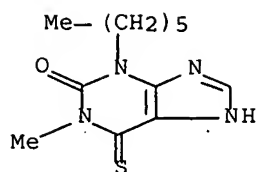
RN 42458-95-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(3-methylbutyl)-6-thioxo- (9CI) (CA INDEX NAME)



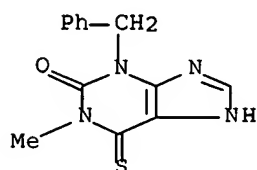
RN 42458-96-8 CAPLUS

CN 2H-Purin-2-one, 3-hexyl-1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



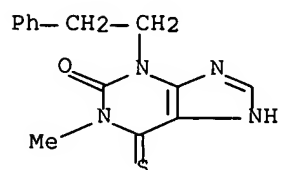
RN 42458-97-9 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(phenylmethyl)-6-thioxo-  
(9CI) (CA INDEX NAME)



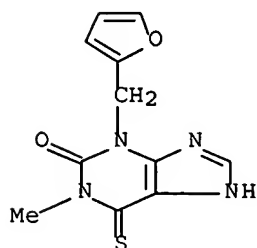
RN 42458-98-0 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-phenylethyl)-6-thioxo-  
(9CI) (CA INDEX NAME)



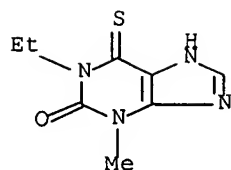
RN 42458-99-1 CAPLUS

CN 2H-Purin-2-one, 3-(2-furanylmethyl)-1,3,6,7-tetrahydro-1-methyl-6-thioxo-  
(9CI) (CA INDEX NAME)



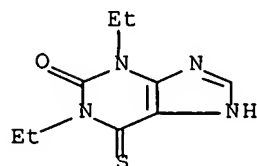
RN 42459-00-7 CAPLUS

CN 2H-Purin-2-one, 1-ethyl-1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA  
INDEX NAME)



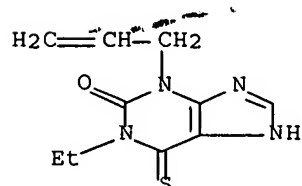
RN 42459-01-8 CAPLUS

CN 2H-Purin-2-one, 1,3-diethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



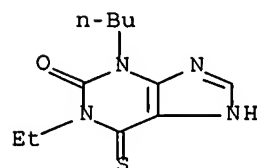
RN 42459-02-9 CAPLUS

CN 2H-Purin-2-one, 1-ethyl-1,3,6,7-tetrahydro-3-(2-propenyl)-6-thioxo- (9CI) (CA INDEX NAME)



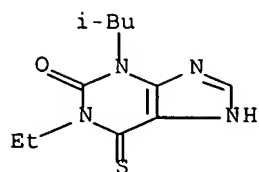
RN 42459-03-0 CAPLUS

CN 2H-Purin-2-one, 3-butyl-1-ethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



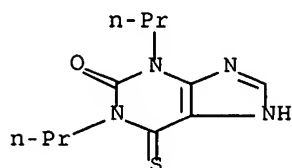
RN 42459-04-1 CAPLUS

CN 2H-Purin-2-one, 1-ethyl-1,3,6,7-tetrahydro-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



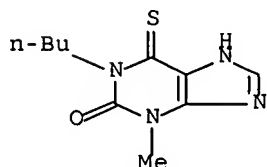
RN 42459-06-3 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dipropyl-6-thioxo- (9CI) (CA INDEX NAME)



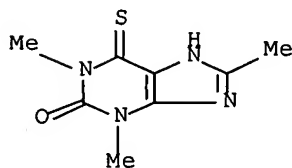
RN 42459-07-4 CAPLUS

CN 2H-Purin-2-one, 1-butyl-1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



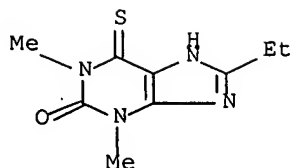
RN 42459-09-6 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3,8-trimethyl-6-thioxo- (9CI) (CA INDEX NAME)

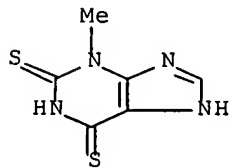


RN 42459-10-9 CAPLUS

CN 2H-Purin-2-one, 8-ethyl-1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 71 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1973:136229 CAPLUS Full-text  
 DOCUMENT NUMBER: 78:136229  
 TITLE: Tautomerism, protonation, and methylation in (methylthio)purines. Factors determining electrophilic attack on purines  
 AUTHOR(S): Reichman, Uri; Bergmann, Felix; Lichtenberg, Dov; Neiman, Zohar  
 CORPORATE SOURCE: Dep. Pharmacol., Heb. Univ., Jerusalem, Israel  
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1973), No. 8, 793-800  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 12 May 1984  
 AB The predominant tautomers, the position of protonation in aqueous solution, and the course of methylation in aprotic solvents were determined for all the mono- and bis(methylthio)purines and for 2,6,8,-tris(methylthio)purine. Protonation gave resonating cations in which the charge is distributed over both rings. 8-(Methylthio)- and 2,8-bis(methylthio)purine underwent methylation at N-1. 6-(Methylthio)-, 6,8-bis(methylthio)-, and 2,6,8-tris(methylthio)purine gave N-3 Me derivs. Methylation of 2-(methylthio)- and 2,6-bis(methylthio)purine occurred at both N-7 and N-9. The results were explained in terms of electronic and steric factors  
 IT 33285-77-7  
 RL: RCT (Reactant); RACT (Reactant or reagent) (methylation of)  
 RN 33285-77-7 CAPLUS  
 CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)



L57 ANSWER 72 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1973:72173 CAPLUS Full-text  
 DOCUMENT NUMBER: 78:72173  
 TITLE: Cephalosporins  
 INVENTOR(S): Sugimoto, Keiichi; Kobayashi, Kunio; Nishijima, Kouji; Morimoto, Shiro  
 PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd.

SOURCE: Ger. Offen., 43 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2225694	A	19721214	DE 1972-2225694	19720526 <--
DE 2225694	B2	19750410		
DE 2225694	C3	19751120		
JP 51016436	B	19760524	JP 1971-38007	19710531 <--
AU 7242504	A	19731122	AU 1972-42504	19720519 <--
ES 403305	A1	19750501	ES 1972-403305	19720530 <--
BE 784181	A1	19721130	BE 1972-4069	19720531 <--
NL 7207368	A	19721204	NL 1972-7368	19720531 <--
FR 2140133	A1	19730112	FR 1972-19538	19720531 <--
HU 164340	B	19740128	HU 1972-TA1189	19720531 <--
GB 1348737	A	19740320	GB 1972-25417	19720531 <--
AT 316746	B	19740725	AT 1972-4720	19720531 <--
AT 318810	B	19741125	AT 1973-4101	19720531 <--
US 3872115	A	19750318	US 1972-258177	19720531 <--
			JP 1971-38007	A 19710531 <--

## PRIORITY APPLN. INFO.:

ED Entered STN: 12 May 1984

GI For diagram(s), see printed CA Issue.

AB 3-(Heterocyclic methyl)ceph-3-em derivs. [I; R = 5-R2-6-R3-1,2-dihydro-2-oxo-4-pyrimidinyl (R2 = H, NH2, Me, OH, CO2H, R3 = H, OH, NMe2, CO2H), 2-oxopurin-6-yl; R1 = PhCHR4 (R4 = H, NH2, HO3S, HO, H2NCO), cyclohexylmethyl, PhSCH2, 1-tetrazolylmethyl, EtCHBr, NCCH2, PhOCH2] were prepared by treating the corresponding cephalosporanic acid with a heterocyclic mercaptol. Thus, Na 7-(2-thienylacetamido)cephalosporanate was treated with 4-thiopyrimidin-2-one in Me2SO to give I (R = 1,2-dihydro-2-oxo-4-pyrimidinyl, R1 = 2-thienyl).

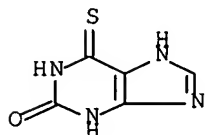
IT 39879-29-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with sodium acetoxymethyl(thienylacetamido)cephalosporanate)

RN 39879-29-3 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-6-thioxo-, monoammonium salt (9CI) (CA INDEX NAME)



● NH3

L57 ANSWER 73 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1972:513624 CAPLUS Full-text

DOCUMENT NUMBER: 77:113624

TITLE: Tautomerism and ionization processes in 6-thioxanthine and its N-methyl derivatives



AUTHOR(S): Lichtenberg, D.; Bergmann, F.; Neiman, Z.  
 CORPORATE SOURCE: Dep. Pharm., Heb. Univ., Jerusalem, Israel  
 SOURCE: Journal of the Chemical Society, Perkin Transactions  
 2: Physical Organic Chemistry (1972-1999) (1972), (11), 1676-81  
 CODEN: JCPKBH; ISSN: 0300-9580

DOCUMENT TYPE: Journal  
 LANGUAGE: English

ED Entered STN: 12 May 1984

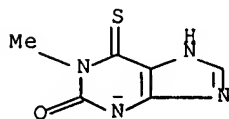
GI For diagram(s), see printed CA Issue.

AB Uv and PMR spectra were recorded of 6-thioxanthine and 10 of its N-Me derivs.; spectra were also obtained of some of their mono- and dianionic and cationic forms. In aqueous solns. of thioxanthines with a free NH in the imidazole ring the 7-NH-tautomer (I) predominated. The order of NH-group acidities was  $3 > 7 > 1$ . The anions of 6-thioxanthine and its 1-Me derivative tautomerized to the NH form. Interactions between H and Me groups at positions 3 and 9 were indicated by the pK values of the 9-methylthioxanthines and by the large downfield displacement of the PMR signals of the 3- and 9-Me groups in 3,9-dimethylthioxanthines.

IT 38759-09-0 38759-10-3 38759-11-4  
 38759-12-5 38759-18-1 38759-19-2  
 38800-21-4 38814-97-0 38814-98-1  
 38814-99-2 38887-43-3  
 RL: PRP (Properties)  
 (NMR and uv spectrum of)

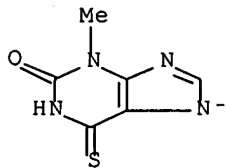
RN 38759-09-0 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-6-thioxo-, ion(1-) (9CI) (CA INDEX NAME)



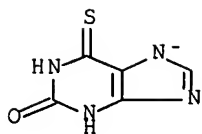
RN 38759-10-3 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo-, ion(1-) (9CI) (CA INDEX NAME)



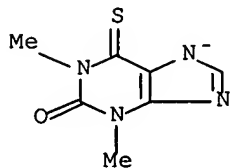
RN 38759-11-4 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-6-thioxo-, ion(1-) (9CI) (CA INDEX NAME)



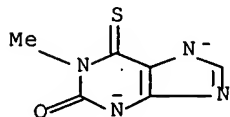
RN 38759-12-5 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo-, ion(1-) (9CI)  
(CA INDEX NAME)



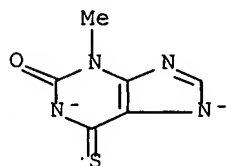
RN 38759-18-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-6-thioxo-, ion(2-) (9CI) (CA  
INDEX NAME)



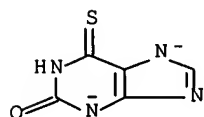
RN 38759-19-2 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo-, ion(2-) (9CI) (CA  
INDEX NAME)



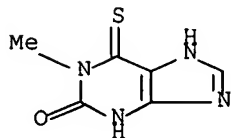
RN 38800-21-4 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-6-thioxo-, ion(2-) (9CI) (CA INDEX  
NAME)



RN 38814-97-0 CAPLUS

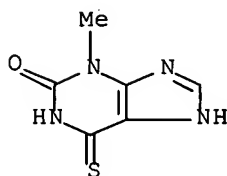
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-6-thioxo-, conjugate monoacid  
(9CI) (CA INDEX NAME)



● H<sup>+</sup>

RN 38814-98-1 CAPLUS

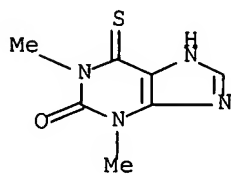
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo-, conjugate monoacid  
(9CI) (CA INDEX NAME)



● H<sup>+</sup>

RN 38814-99-2 CAPLUS

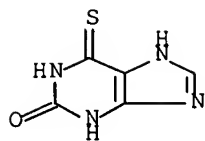
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo-, conjugate monoacid (9CI) (CA INDEX NAME)



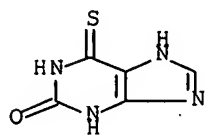
● H<sup>+</sup>

RN 38887-43-3 CAPLUS

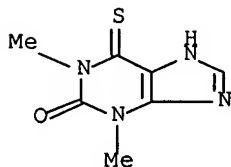
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-6-thioxo-, conjugate monoacid (9CI)  
(CA INDEX NAME)



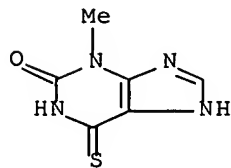
IT 2002-59-7 2398-70-1 33285-76-6  
 38695-85-1  
 RL: PRP (Properties)  
 (ionization and tautomerism of)  
 RN 2002-59-7 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



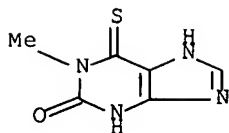
RN 2398-70-1 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 33285-76-6 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 38695-85-1 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 74 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1971:493013 CAPLUS Full-text  
 DOCUMENT NUMBER: 75:93013  
 TITLE: Photographic silver halide materials supersensitized  
 with a combination of a triazole and a cyanine dye  
 INVENTOR(S): Brooks, Dugald A.  
 PATENT ASSIGNEE(S): Eastman Kodak Co.  
 SOURCE: U.S., 6 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3592656	A	19710713	US 1968-757147	19680903 <--
BE 738386	A	19700216	BE 1969-738386	19690903 <--
FR 2020524	A5	19700717	FR 1969-29985	19690903 <--
GB 1282032	A	19720719	GB 1969-1282032	19690903 <--
PRIORITY APPLN. INFO.:			US 1968-757147	A 19680903 <--

ED Entered STN: 12 May 1984

AB Photog. Ag halide emulsions were supersensitized by a combination of a sensitizing methine dye and pyrazolone, triazole, tetrazole, or imidazole. For example, a Ag(Br,I) emulsion containing 80 mg 3,3'-diethyl-4,5,4',5'-naphthoselenadicarbocyanine iodide/mole Ag and 0.3-10g 3-(3,4-dichloroanilino)-1-(2,4,6-trichlorophenyl)-5-pyrazolone/mole Ag was exposed and gave a relative speed 692 compared to 100 for a similar emulsion containing no pyrazolone.

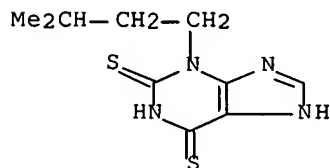
IT 32051-91-5

RL: USES (Uses)

(photographic supersensitizers from cyanine dyes and)

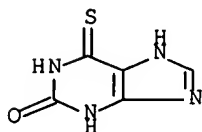
RN 32051-91-5 CAPLUS

CN Xanthine, 3-isopentyl-2,6-dithio- (7CI, 8CI) (CA INDEX NAME)

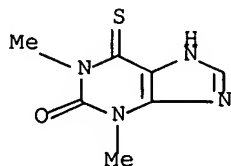


L57 ANSWER 75 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1971:434696 CAPLUS Full-text

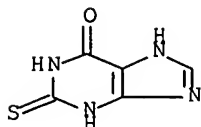
DOCUMENT NUMBER: 75:34696  
 TITLE: Nuclear magnetic resonance spectra of xanthines and thioxanthines  
 AUTHOR(S): Bergmann, F.; Lichtenberg, D.; Neiman, Z.  
 CORPORATE SOURCE: Hadassah Med. Sch., Heb. Univ., Jerusalem, Israel  
 SOURCE: Journal of the Chemical Society [Section] C: Organic (1971), (10), 1939-41  
 CODEN: JSOOAX; ISSN: 0022-4952  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 12 May 1984  
 AB The NMR signal of the 8-H in xanthines is shifted downfield more strongly by introduction of a 2- than of a 6-thioxo group. The signals of N-Me groups are also shifted to lower field, but the effect depends strictly on the distance between the Me and the thioxo. In 2-thioxanthines, the displacement decreases in the order 1-Me = 3-Me > 7-Me, and in 6-thioxanthines the sequence is 1-Me > 7-Me > 3-Me > 9-Me.  
 IT 2002-59-7 2398-70-1 2487-40-3  
 5437-25-2 6501-94-6 6603-63-0  
 28139-02-8 33285-76-6 33285-77-7  
 RL: PRP (Properties)  
 (nuclear magnetic resonance of)  
 RN 2002-59-7 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



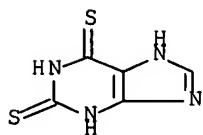
RN 2398-70-1 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



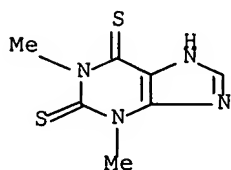
RN 2487-40-3 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



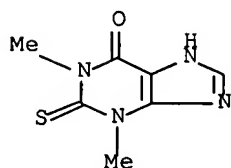
RN 5437-25-2 CAPLUS  
 CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



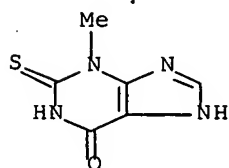
RN 6501-94-6 CAPLUS  
 CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



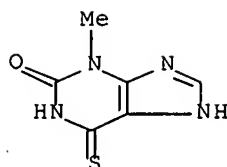
RN 6603-63-0 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



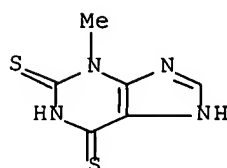
RN 28139-02-8 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



RN .33285-76-6 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)

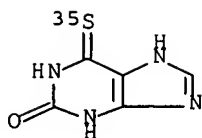


RN 33285-77-7 CAPLUS  
 CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)



L57 ANSWER 76 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1971:125639 CAPLUS Full-text  
 DOCUMENT NUMBER: 74:125639  
 TITLE: Sulfur-35 labeling of some organic compounds by a dry method  
 AUTHOR(S): Chiotan, Constantin; Zamfir, Ioana; Szabo, Maria; Turcanu, Cornelius N.  
 CORPORATE SOURCE: Inst. At. Phys., Bucharest, Rom.  
 SOURCE: Nov. Metody Poluch. Radioaktiv. Prep., Sb. Dokl. Simp. (1970), Meeting Date 1969, 386-401.  
 Postoyan. Kom. Ispol'z. At. Energ. Mirnykh Tselyakh: Warsaw, Pol.  
 CODEN: 22YYAY  
 DOCUMENT TYPE: Conference  
 LANGUAGE: Russian  
 ED Entered STN: 12 May 1984  
 AB The S in p-AcNHC6H4CH:NNHCSNH2, (H2N)2CS, PhNHCSNH2, 6-mercaptopurine, and 2-thioxanthine was replaced with 35S by heating at 150-280° with excess elemental 35S. 6-Thioguanine-35S was prepared from the unlabeled compound by acetylation, isotope exchange as above, and hydrolysis. 2-Thiouracil and its 6-Me derivative were labeled by heating at 200 and 250°, resp., with equal quantities of 35S and C10H8; MeC35SNH2 was prepared by this method in refluxing iso-BuOH. Heating sulfanilamide at 180° with (NH4)235SO4 afforded p-H2NC6H435SO2NH2.  
 IT 31494-01-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 31494-01-6 CAPLUS  
 CN Xanthine, 6-thio-35S- (8CI) (CA INDEX NAME)





L57 ANSWER 77 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1971:118381 CAPLUS Full-text  
 DOCUMENT NUMBER: 74:118381  
 TITLE: Silver halide photographic emulsions containing supersensitizing compositions  
 INVENTOR(S): Brooks, Dugald Arthur  
 PATENT ASSIGNEE(S): Eastman Kodak Co.  
 SOURCE: Fr. Demande, 21 pp.  
 CODEN: FRXXBL  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2020524	A5	19700717	FR 1969-29985	19690903 <--
US 3592656	A	19710713	US 1968-757147	19680903 <--
PRIORITY APPLN. INFO.:			US 1968-757147	A 19680903 <--

ED Entered STN: 12 May 1984

AB The title emulsions contain a sensitizing dye in conjunction with a heterocyclic compound such as 5-pyrazolone, 1,2,3,4-tetrazole, 1,2,4-triazole, imidazole, or an imidazolinium salt. E.g., a gelatin Ag(Br,I) (0.77 mole % AgI) emulsion was combined with 80 mg 5-[bis[1-ethyl-2(1H)- $\beta$ -naphthothiazolylylidene]isopropylidene] - 1,3 - bis( $\beta$  - methoxyethyl)barbituric acid per mole Ag halide and with 0.66 g 1,5-diphenyl-1,2,4-triazole (I) per g atom Ag. The emulsion was ripened for 10 min at 50°, coated on a cellulose acetate support to give 46 mg Ag/dm<sup>2</sup>, and sensitometrically tested. A similar material without I was tested for comparison. The relative sensitivity of both materials was 75,900 and 100, resp.,  $\gamma$  1.50 and 1.33, and fog 0.06 and 0.05.

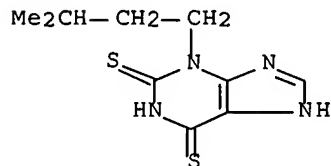
IT 32051-91-5

RL: USES (Uses)

(photographic supersensitizers from carbocyanine dyes and)

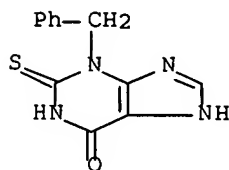
RN 32051-91-5 CAPLUS

CN Xanthine, 3-isopentyl-2,6-dithio- (7CI, 8CI) (CA INDEX NAME)



L57 ANSWER 78 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1970:466537 CAPLUS Full-text

DOCUMENT NUMBER: 73:66537  
 TITLE: N .far. N alkyl and glycosyl migration of purines and pyrimidines. III. N .far. N alkyl and glycosyl migration of purine derivatives  
 AUTHOR(S): Miyaki, Michiko; Shimizu, Bunji  
 CORPORATE SOURCE: Cent. Res. Lab., Sankyo Co., Ltd., Tokyo, Japan  
 SOURCE: Chemical & Pharmaceutical Bulletin (1970), 18(7), 1446-56  
 CODEN: CPBTAL; ISSN: 0009-2363  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 73:66537  
 ED Entered STN: 12 May 1984  
 AB Alkyl and glycosyl migration reactions of N1-, N3-, N7-, and N9-substituted derivs. of adenine, N6,N6-dimethyladenine, N2-acetylguanine, and purine were demonstrated. The NMR chemical shifts of these derivs. were determined and the frontier  $\pi$ -electron ds. of nitrogens in purine ring calculated by a simple LCAOMO method. The results provided the order of thermodynamic stability and kinetic effect of the derivs. on the alkylation reaction.  
 IT 28741-76-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 28741-76-6 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-(phenylmethyl)-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 79 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1970:444460 CAPLUS Full-text  
 DOCUMENT NUMBER: 73:44460  
 TITLE: Charge transfer spectra of bases, nucleosides, and nucleotides  
 AUTHOR(S): Saucin, Michel; Van de Vorst, Albert  
 CORPORATE SOURCE: Dep. Phys. At. Mol., Univ. Liege, Sart-Tilman/Liege, Belg.  
 SOURCE: Journal de Chimie Physique et de Physico-Chimie Biologique (1970), 67(3), 507-11  
 CODEN: JCPBAN; ISSN: 0021-7689  
 DOCUMENT TYPE: Journal  
 LANGUAGE: French  
 ED Entered STN: 12 May 1984  
 AB Spectrophotometric investigation was carried out in systems formed by purines, pyrimidines, nucleosides, and nucleotides as donors and chloranil and 1,3,5-trinitrobenzene as acceptor. In some cases, a partial charge transfer is observed which manifests itself by the appearance of a new optical band, but, in general, specific bands of the acceptor's ion were observed, which can be interpreted as the complete transfer of an electron. Most of the mols. are very good electron donors.  
 IT 29373-31-7 29665-67-6

RL: PRP (Properties)  
(spectrum of, uv, charge-transfer band in)

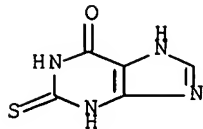
RN 29373-31-7 CAPLUS

CN p-Benzoquinone, 2,3,5,6-tetrachloro-, compd. with 2-thioxanthine (8CI)  
(CA INDEX NAME)

CM 1

CRN 2487-40-3

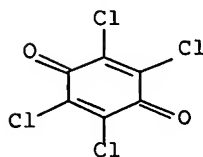
CMF C5 H4 N4 O S



CM 2

CRN 118-75-2

CMF C6 Cl4 O2



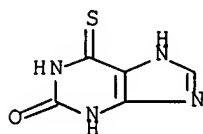
RN 29665-67-6 CAPLUS

CN p-Benzoquinone, 2,3,5,6-tetrachloro-, compd. with 6-thioxanthine (8CI)  
(CA INDEX NAME)

CM 1

CRN 2002-59-7

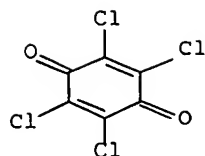
CMF C5 H4 N4 O S



CM 2

CRN 118-75-2

CMF C6 Cl4 O2



L57 ANSWER 80 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1970:403341 CAPLUS Full-text

DOCUMENT NUMBER: 73:3341

TITLE: Dipole moments and electronic structure of some xanthine and thioxanthine derivatives

AUTHOR(S): Weiler-Feilchenfeld, Hannah; Neiman, Zohar

CORPORATE SOURCE: Dep. Org. Chem., Hebrew Univ., Jerusalem, Israel

SOURCE: Journal of the Chemical Society [Section] B: Physical Organic (1970), 4, 596-8

CODEN: JCSPAC; ISSN: 0045-6470

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 12 May 1984

AB The dipole moments and uv absorption spectra of caffeine, theophylline, and their 2-thio-, 6-thio- and 2,6-dithio derivs. were measured. From the differences between the moments of these compounds it can be deduced that the C:S group moment is higher by 1.1 D than that of C:O; the direction of the moment of caffeine forms an angle of 96° counterclockwise with the C(4) → C(5) axis, in good agreement with theoretical predictions.

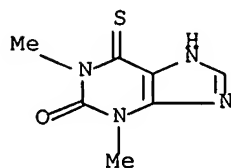
IT 2398-70-1 6501-94-6 6603-63-0

RL: PRP (Properties)

(dipole moment of)

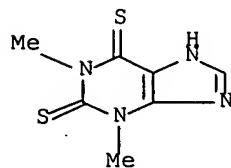
RN 2398-70-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)

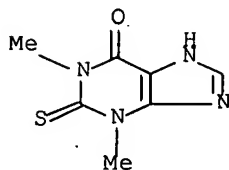


RN 6501-94-6 CAPLUS

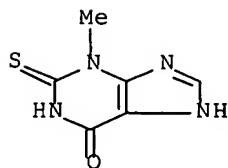
CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



RN 6603-63-0 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 81 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1970:126337 CAPLUS Full-text  
 DOCUMENT NUMBER: 72:126337  
 TITLE: Mass spectrometric investigations of heterocyclic compounds. V. Fragmentation of some purines  
 AUTHOR(S): Heiss, Juergen; Zeller, Klaus P.; Voelter, Wolfgang  
 CORPORATE SOURCE: Chem. Inst., Univ. Tuebingen, Tuebingen, Fed. Rep. Ger.  
 SOURCE: Organic Mass Spectrometry (1970), 3(2), 181-90  
 CODEN: ORMSBG; ISSN: 0030-493X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 ED Entered STN: 12 May 1984  
 AB The mass spectra of 9 purines are discussed. The xanthine purines eliminate HNCO and CO consecutively, whereas 3-methylhypoxanthine loses HCN and CO. In the case of 3-methylxanthine, an ion is formed whose stabilization by rearrangement is discussed. The fragmentation patterns of 3-methyl-2-thioxanthine and 3-methylthiohypoxanthine are different from those of the corresponding O analogs. 6-(Methylthio)purine and 6-methoxypurine eliminate HCS· or HCO·, resp. For the latter reaction a mechanism is suggested.  
 IT 28139-02-8  
 RL: PRP (Properties)  
 (mass spectrum of)  
 RN 28139-02-8 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 82 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1968:496632 CAPLUS Full-text  
 DOCUMENT NUMBER: 69:96632  
 TITLE: Reactions of 4,5-diaminouracils with  $\beta$ -oxoesters  
 AUTHOR(S): Stahl, P. H.; Merz, K. W.

CORPORATE SOURCE: Univ. Freiburg/Br., Freiburg/Br., Fed. Rep. Ger.  
 SOURCE: Pharmazie (1967), 22(11), 630-4  
 CODEN: PHARAT; ISSN: 0031-7144

DOCUMENT TYPE: Journal  
 LANGUAGE: German

ED Entered STN: 12 May 1984

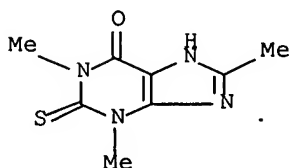
GI For diagram(s), see printed CA Issue.

AB 5,6-Diamino-1,3-dimethyluracil (I) refluxed with an equimol. amount of AcCH<sub>2</sub>CO<sub>2</sub>Et gave 80% II (X = Y = O, R = Me), decompose 216-19°; 2,4-dinitrophenylhydrazones m. 255-8°. Following II were prepared (X, Y, R, m.p., m.p. after resolidification, and m.p. of 2,4-dinitrophenylhydrazones given): O, O, Ph, 250-2°, 310-40°, 268-70°; O, O, 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, 259-63°, 360°, -; O, O, pyridin-3-yl, 260-3°, 245°, 261-2°; O, O, α-furyl, 224-32°, -, -; O, S, Me, 225-8°, -, -; S, S, Me, 212°, -, -; O, S, Ph, 223-9°, -, -; S, O, pyridin-3-yl, 257-63°, -, -; O, S, pyridin-3-yl, 244-53°, -, -; S, O, 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, 230-5°, 290-300°, -; O, S, 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, 240-2°, -, -; S, S, 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, 225°, -, -. 1,3-Dimethyl-4,5-diamino-2-thiouracil (3.7 g.) and 2.6 g. AcCH<sub>2</sub>CO<sub>2</sub>Et refluxed in xylene 5 hrs. gave 86% 2,3,6,7,8,9-hexahydro-4,6,8-trimethyl-7-thio-2,9-dioxo-1H-pyrimido[4,5b] - 1,5-diazepine, m. 240-90°, which was converted into 1,3-dimethyl-4-amino-5-(acetoacetyl amino)-2-thiouracil; 2,4-dinitrophenylhydrazones m. 245-7°. Also prepared was 1,3-dimethyl-4-amino-5-(1-ethoxycarbonyl-2-propylideneamino)-2-thiouracil, m. 210-22° (after resolidification m. 320-30°), which, heated to 250° and treated with NaOH gave 44% 8-methyl-2-thiotheophylline, m. 340-3°. I (2.55 g.) refluxed with 10 g. AcCH<sub>2</sub>CO<sub>2</sub>Et in 100 ml. PhNO<sub>2</sub> gave 45.4% 8-methyltheophylline, m. 330°; picrate m. 282-305°.

IT 19673-55-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 19673-55-3 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3,8-trimethyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 83 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1968:459201 CAPLUS Full-text

DOCUMENT NUMBER: 69:59201

TITLE: Selective removal of the benzyl group from position 3 of purines

AUTHOR(S): Neiman, Z.; Bergmann, F.

CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel

SOURCE: Israel Journal of Chemistry (1968), 6(1), 9-16  
 CODEN: ISJCAT; ISSN: 0021-2148

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 12 May 1984

GI For diagram(s), see printed CA Issue.

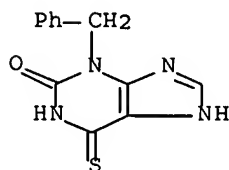
AB 3-Benzyl-7-methyl-6-thiopurine (I) is treated with HBr to give 7-methyl-6-thiopurine (II). Also prepared are 3-benzyl-2-thiouric acid (III) and IV. Thus, a mixture of 1 g. 3-benzyl-6-(methylthio)purine, 50 ml. MeCN, and 10 ml. MeI is refluxed 1 hr. to give 60% I, m. 220-5° (decomposition). A mixture of 1 g. 1-benzyl-5,6-diamino-4-hydroxy-2-thiopyrimidine and 3 g. urea is heated 30 min. at 180° to give III, m. >300° (HOAc); a mixture of 10 g. III, 700 ml. 3% NH<sub>3</sub>, and 100 g. Raney Ni is refluxed 2 hrs. to give 56% 3-benzyl-6,8-dihydroxypurine [IV (R = CH<sub>2</sub>Ph)] (V), m. >280° (HOAc). Similarly prepared is 3-benzyl-2-oxopurine, m. >240° (decomposition) (MeCN). A solution of 0.5 g. 3-benzyl-2-thioxanthine in 10N NaOH is heated to 50° and 1.5 ml. 30% H<sub>2</sub>O<sub>2</sub> is slowly added to give 41% 3-benzylxanthine (VI), m. >300° (decomposition); a mixture of 1 g. VI, 3 g. P<sub>2</sub>S<sub>5</sub>, and 100 ml. pyridine is refluxed 4 hrs. to give 75% 3-benzyl-6-thioxanthine, m. >250° (decomposition). Uv data are given. Solns. of 1 g. I (and V) in 30 ml. 48% HBr are boiled 3-5 min. to give 75-90% II and IV (R = H).

IT 19844-94-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 19844-94-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(phenylmethyl)-6-thioxo- (9CI) (CA  
INDEX NAME)



L57 ANSWER 84 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1967:403051 CAPLUS Full-text

DOCUMENT NUMBER: 67:3051

TITLE: 6-Thioxanthines

AUTHOR(S): Seyden-Penne, Jacqueline; Le Thi Minh; Chabrier, Pierre

CORPORATE SOURCE: Fac. Med., Inst. Pharmacol., Paris, Fr.

SOURCE: Bulletin de la Societe Chimique de France (1966), (12), 3934-38

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal

LANGUAGE: French

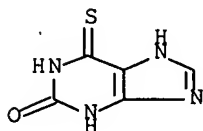
OTHER SOURCE(S): CASREACT 67:3051

ED Entered STN: 12 May 1984

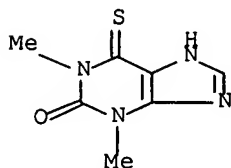
AB The reaction of 6-thiotheophyllines (I) with alkyl halides in different solvents has been examined. Dry Na theophyllinate refluxed in anhydrous EtOH with an equimol. quantity of 2-chloro- and 2-bromoethanol gave a precipitate of the alkaline metal halide; on cooling the I crystallizes. In anhydrous HCONMe<sub>2</sub> in the presence of NaH or K<sub>2</sub>CO<sub>3</sub>, only gums or the original material were obtained, depending on the temperature and reaction time. I and epoxide, in the presence of C<sub>5</sub>H<sub>5</sub>N, refluxed in anhydrous PROH gave 7-(β-alkyl-β-hydroxyethyl)-6-thiotheophyllines in poor yields. By replacing PROH by HCONMe<sub>2</sub>, an aprotic polar solvent which favors anionic nucleophilic substitution, the yields were appreciably increased. Thus, I (0.05 moles), 2 ml. C<sub>5</sub>H<sub>5</sub>N, and 80 ml. HCONMe<sub>2</sub> in which were dissolved 0.125 moles ethylene oxide, kept 3 hrs. at 100° in a sealed tube, gave 50% 7-(β-hydroxyethyl)-6-

thiotheophylline, m. 137°. 7-( $\beta$ -Hydroxypropyl)-6-thiotheophylline, m. 165°, 7-( $\beta,\gamma$ -dimethoxypropyl)-6-thiotheophylline, m. 137°, and 7-( $\gamma$ -chloro- $\beta$ -hydroxypropyl)-6-thiotheophylline, m. 175° were similarly prepared in 50-60% yields. The structure of these compds. was confirmed by uv, ir, and N.M.R. spectra. Desulfurization of these compds. was confirmed by uv, ir, and N.M.R. spectra. Desulfurization of these compds. was accomplished using Raney Ni, rich in H, freshly prepared at temps. below 60°, by refluxing in EtOH at 96° and renewing the catalyst every hr. Thus, the following 1,3-dimethyl-2-oxo-7-alkyl-1,2,3,6-tetrahydropurines were obtained (alkyl group and m.p. given): CH<sub>2</sub>CH<sub>2</sub>OH, 210°; CH<sub>2</sub>CHOHCH<sub>3</sub>, 224°, CH<sub>2</sub>CHOHCH<sub>2</sub>OH, 240°. The uv, ir, and N.M.R. spectra of the desulfurized compds. were examined and compared to those of the alkylated I.

IT 2002-59-7DP, Xanthine, 6-thio-, derivs. 2398-70-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 2002-59-7 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



RN 2398-70-1 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 85 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1967:2448 CAPLUS Full-text  
 DOCUMENT NUMBER: 66:2448  
 TITLE: Oxidation products of thiocarboxylic acid amides.  
 XII. Oxidation reactions of thiolimide esters and  
 N-heteroaromatic compounds with  $\alpha$ - and  
 $\gamma$ -thiocarbonyl groups  
 AUTHOR(S): Walter, Wolfgang; Voss, Juergen; Curts, Julius  
 CORPORATE SOURCE: Univ. Hamburg, Hamburg, Germany  
 SOURCE: Justus Liebig's Annalen der Chemie (1966),  
 695, 77-86  
 CODEN: JLACBF; ISSN: 0075-4617  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 OTHER SOURCE(S): CASREACT 66:2448  
 ED Entered STN: 12 May 1984  
 GI For diagram(s), see printed CA Issue.



AB cf. CA 65, 13501a. Thioliimide esters 4-R1C6H4C(SR3):NC6H4R2-4 (I) are oxidized by BzOOH to the corresponding amides 4-R1C6H4CONHC6H4R2-4 (R1 and R2 same as in I) (II). 2- (III) and 4-pyridinethione (IV) and purine-6-thione (V) give with H2O2 S-oxides, which however easily react further to give disulfides, and in basic medium to give sulfonic acids. Oxidns. of other N-heteroaromatic compds. are reported. An EtOH solution of the appropriate Na thiophenolate treated with an equivalent amount appropriate imide chloride in Et2O, after 12 hrs. at room temperature the solution filtered and evaporated, and the residue recrystd. from EtOH gave approx. 50% I. The following were prepared (R1, R2, R3, m.p., m.p. corresponding II (R1 and R2 same as in I) given): H, H, Me, 63-4°, 165-6°; H, H, Ph (VI), 54-6°, 165-6°; H, H, C6H4NO2-4 (VII), 81-4°, 165-6°; H, NO2, Ph, 108-9°, 201-2°; NO2, H, Ph, 67-8°, 213-15°; H, OMe, Ph, 64-5°, 155-7°; MeO, H, Ph, 65-6°, 175-6°; MeO, OMe, Ph, 95-6°, 204°; MeO, OMe, C6H4NO2-4, 129-31°, 204°. The appropriate I (0.1 mole) and 0.2 mole 30% H2O2 were dissolved in CHCl3 under external cooling, after 12 hrs. at room temperature, the precipitate (A) filtered off, the filtrate washed with aqueous NaHCO3, dried, and evaporated, and the residue recrystd. from EtOH with C to give the corresponding II, m.ps. being shown in the first table; in 2 cases (VI and VII) the precipitate A was identified as (PhNH3)+(O3SC6H4R)- (VIII) (R = H) and VIII (R = NO2), resp. 2-Benzylsulfinylpyridine (IX) [obtained from 2-benzylthiopyridine (X)] (1.17 g.) in 35 cc. CHCl3 kept 70 hrs. at room temperature with 0.87 g. BzOOH and the solution washed with aqueous Na2CO3, dried, and evaporated gave 0.78 g. 2-benzylsulfonylpyridine (Xa), m. 114-15° (EtOAc-petr. ether). X N-oxide (0.50 g.) and 0.34 g. BzOOH in 15 cc. CHCl3 kept 3 days at room temperature and worked up like Xa gave 0.30 g. IX N-oxide (XI), m. 119° (EtOAc-petr. ether). XI (0.47 g.) and 0.7 g. BzOOH in 15 cc. CHCl3 kept 2 days at room temperature and worked up like Xa gave 0.35 g. Xa N-oxide, m. 126-8° (EtOAc-petr. ether). 2-Thiazolidinethione (XII) (3 g.) in 150 cc. MeOH and 150 cc. CH2Cl2 treated with 2 cc. 30% H2O2 at room temperature, the solution kept 30 min. and poured into H2O, the aqueous layer separated, extracted twice with CH2Cl2, and treated dropwise with 1.5% MeOHFeCl3 (the aqueous layer was colored deep blue), and the product extracted immediately with CH2Cl2 gave 310 mg. Fe(III) complex (XIII) of XIV, blue, m. 70.5-2.0°; thin layer chromatography (TLC) on silica gel G with 3:1 C6H6-MeOH showed that XIII still contained XII. Similar oxidation of 2-oxazolidinethione gave an aqueous solution of XV, which was detected only in solution with FeCl3 (blue color). III (200 mg.) in 10 cc. CHCl3 and 5 cc. EtOH treated with 0.5 cc. 30% H2O2 and the yellow solution treated with 1% EtOH-FeCl3 gave a blue green color [indicative of III S-oxide (XVI)], which rapidly faded; after 15 min. XVI was no longer detectable. Treatment of 200 mg. IV in 10 cc. HCONMe2 (DMF) with 1 cc. 30% H2O2 gave the same result as with III. N-Methyl-2-pyridinethione (XVIa) (200 mg.) in 10 cc. CHCl3 and 10 cc. EtOH treated with 0.12 cc. 30% H2O2 and then with FeCl3 gave an olive green-blue color; on TLC on silica gel with EtOAc, the FeCl3-pos. substance remained at the starting point. III (6.7 g.) in 100 cc. MeOH kept 40 min. with 7.2 cc. 30% H2O2 and evaporated gave 4.8 g. bis(2-pyridyl) disulfide, m. 57° (6:7 C6H6-petr. ether); picrate m. 119° (EtOH). IV (200 mg.) in 10 cc. DMF kept 1 hr. with 0.5 cc. 30% H2O2 and diluted with H2O deposited 0.1 g. bis(4-pyridyl) disulfide, m. 77° (6:7 C6H6-petr. ether); picrate m. 225° (decomposition) (DMF). XVIa (100 mg.) in 3 cc. MeOH treated with 0.2 cc. Et3N and 0.3 cc. 30% H2O2, kept 5 min., and examined by TLC (silica gel, EtOAc) showed the presence of XVIa (Rf 0.41), XVIa S-oxide (Rf 0.00), and N-methyl-2-pyridone (Rf 0.10), which could be detected with iodine-azide reagent and with FeCl3 (red color). III (1.1 g.) in 50 cc. 2N NaOH kept 50 min. with 5% 30% H2O2, acidified with 2N HCl, neutralized with aqueous NaHCO3, and evaporated, the residue extracted with boiling MeOH, and the extract evaporated gave 1.25 g. Na 2-pyridine-sulfonate (XVII), m. >300° (EtOH-H2O), identical (ir spectrum) with authentic XVII. From IV was similarly obtained 11% Na 4-pyridinesulfonate (XVIII), m. >300°, identical (ir spectrum) with authentic XVIII. XVIa (0.25 g.) in 25 cc. CHCl3 and 25 cc.

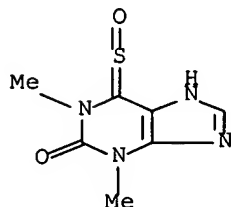
EtOH heated 10 min. at 50° with 1 cc. 30% H<sub>2</sub>O<sub>2</sub> and evaporated and the residual sirup kept 3 days at -20° gave 10 mg. XIX, m. 265°, identical (ir spectrum) with authentic XIX. Investigation of S-oxide formation with V and substituted V by H<sub>2</sub>O<sub>2</sub> gave the following results [starting compound, solvent, FeCl<sub>3</sub> reaction, R<sub>f</sub> value (TLC on silica gel G with 3:1 C<sub>6</sub>H<sub>6</sub>-MeOH) given]: V, Me<sub>2</sub>SO, blue (indicative of S-oxide formation), -; 1-Me derivative (XX) of V, MeOH-CHCl<sub>3</sub> + Et<sub>3</sub>N, blue (indicative of S-oxide formation), 0.07; 6-thiotheobromine, DMF, blue (indicative of S-oxide formation), 0.00; 2-imino derivative of XX, no S-oxide detectable, -; 6-thiocaffeine (XXI), no S-oxide detectable, -. 6-Thiotheophylline (200 mg.) and 1 cc. Et<sub>3</sub>N in 50 cc. CHCl<sub>3</sub> and 50 cc. EtOH kept 15 min. at 50° with 1 cc. 30% H<sub>2</sub>O<sub>2</sub>, concentrated as rapidly as possible in vacuo at <30° (bath) until crystallization began, and cooled at -20° gave 158 mg. S-oxide hydrate (XXII.H<sub>2</sub>O), m. 241-5° (decomposition), R<sub>f</sub> 0.29 (TLC on silica gel G with 3:1 C<sub>6</sub>H<sub>6</sub>-MeOH); the stability of XXII was attributed to intramol. H bridge formation. XXI (500 mg.) in 15 cc. AcOH heated with 3 cc. 30% H<sub>2</sub>O<sub>2</sub> at 50° (transient deep yellow color formed, but no S-oxide was detectable with FeCl<sub>3</sub>), after 5 min. the solution diluted with 150 cc. H<sub>2</sub>O, excess H<sub>2</sub>O<sub>2</sub> destroyed with MnO<sub>2</sub>, and the solution filtered, concentrated, neutralized with aqueous NH<sub>3</sub>, and extracted 3 times with CHCl<sub>3</sub> gave, from the exts., caffeine, m. 239° (EtOH). V (300 mg.) in 10 cc. DMF kept 90 min. at 30-5° with 1 cc. 30% H<sub>2</sub>O<sub>2</sub>, diluted with H<sub>2</sub>O, and cooled deposited 130 mg. bis(6-puriny) disulfide (XXIII), identical (TLC on silica gel G with 2:1 C<sub>6</sub>H<sub>6</sub>-EtOH) with authentic XXIII. Ir data were given for some compds.

IT 14156-64-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 14156-64-0 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-sulfinyl- (9CI) (CA  
INDEX NAME)



L57 ANSWER 86 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:420841 CAPLUS Full-text

DOCUMENT NUMBER: 65:20841

ORIGINAL REFERENCE NO.: 65:3877f-h,3878a-c

TITLE: Purine derivatives. III. Sulfur-containing  
theophyllines. I

AUTHOR(S): Merz, K. W.; Stahl, P. H.

CORPORATE SOURCE: Univ. Freiburg/Br., Germany

SOURCE: Beitr. Biochem. Physiol. Naturstoffen, Festschr. (1965) 285-98

DOCUMENT TYPE: Journal

LANGUAGE: German

ED Entered STN: 22 Apr 2001

GI For diagram(s), see printed CA Issue.

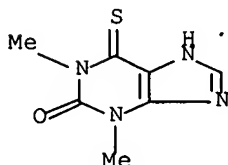
AB cf. CA 63, 4296b. It is easy to prepare 6-thiotheophylline (I) by heating theophylline with P<sub>4</sub>S<sub>10</sub> in a pyridine base b. 140-60° but 2,6-dithiotheophylline (II) can only be prepared (in very small quantities) from

theophylline by melting it together with P4S10. 2-Thiotheophylline (III) was prepared first. Ethyl cyanoacetate, N,N'-dimethylthiourea, and NaOMe was refluxed 15 hrs. in a mol. ratio of 1.5:1:1.5 to give 34.5% 1,3-dimethyl-4-amino-2-thiouracil (IV), m. 289-90°. IV suspended in H<sub>2</sub>O and AcOH, or in HCONH<sub>2</sub>, was cooled in ice and NaNO<sub>2</sub> added dropwise to give blue-green 1,3-dimethyl-4-amino-5-nitroso-2-thiouracil (V), m. 218-20°. V was reduced with Na dithionate at 100°, when 2-5 g. IV was used. When 10-30 g. IV was used, Na dithionate was used as starter, but the reduction itself was effected by formic acid. In both cases, 1,3-dimethyl-4,5-diamino-2-thiouracil (VI), m. 240-3°, was formed, and when HCONH<sub>2</sub> was still present, 1,3-dimethyl-4-amino-5-formylamino-2-thiouracil (VII), m. 304-5°, was formed immediately. By heating VII for 0.5 hr., III, m. 344-8°, was formed, from which II, m. 267-9°, was prepared with P4S10 in pyridine with 1% H<sub>2</sub>O. It was not possible to prepare the nitroso compound from the orange 1,3-dimethyl-4-amino-2,6-dithiouracil (VIII), m. 273-5° (prepared from IV with P4S10), or from 1,3-dimethyl-4-amino-6-thiouracil (IX), m. 283-6° because of the lower electronegativity of the S, compound with the original O. By boiling 1,3-dimethyl-4,5-diaminouracil (X) or VI 12 hrs. with P4S10 in pyridine, 1,3-dimethyl-4,5-diamino-6-thiouracil (XI), and 1,3-dimethyl-4,5-diamino-2,6-dithiouracil (XII) were prepared, resp. With formamide the ring was closed and I, m. 311°, and II, were formed. From VI in stoichiometric ratio with HNO<sub>2</sub> 4,5,6,7-tetrahydro-4,6-dimethyl-5-thio-7-oxo-v-triazolo[4,5-d]pyrimidine (XIII), m. 229°, was obtained; this was not possible with XI and XII. The S in III and I was substituted by 2H, by boiling the compound with Raney Ni in a dilute NH<sub>3</sub> solution, to give 1,2,3,6-tetrahydro-1,3-dimethyl-6-oxopurine (XIV), and 1,2,3,6-tetrahydro-1,3-dimethyl-2-oxopurine (XV), resp., but neither of the S atoms could be substituted in the same way in II. Identification was by thin-layer chromatography on silica gel with 80:12:5 C<sub>6</sub>H<sub>6</sub>-EtOHAcOH. In the uv spectra of the compds. a bathochromic shift of the absorption bands with regard to theophylline was observed. This increased in the order: III, I, II. Also the number of maximum increased, and in methanol solution the intensity of the strongest absorption bands increased in the same order. 21 references.

IT 2398-70-1, Theophylline, 6-thio-  
(potassium derivative)

RN 2398-70-1 CAPLUS

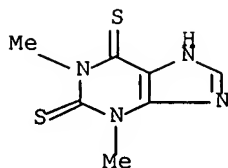
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



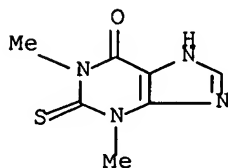
IT 6501-94-6, Theophylline, dithio- 6603-63-0,  
Theophylline, 2-thio-  
(spectrum of)

RN 6501-94-6 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



RN 6603-63-0 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)

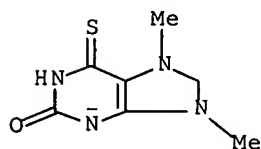


L57 ANSWER 87 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1966:93480 CAPLUS Full-text  
 DOCUMENT NUMBER: 64:93480  
 ORIGINAL REFERENCE NO.: 64:17597b-h,17598a-e  
 TITLE: Syntheses in the purine series. XVII. Syntheses of N,S-purinium betaines  
 AUTHOR(S): Bredereck, Hellmut; Schellenberg, Peter; Nast, Roland; Heise, Hartmut; Christmann, Otto  
 CORPORATE SOURCE: Tech. Hochsch., Stuttgart, Germany  
 SOURCE: Chemische Berichte (1966), 99(3), 944-57  
 CODEN: CHBEAM; ISSN: 0009-2940  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 OTHER SOURCE(S): CASREACT 64:93480  
 ED Entered STN: 22 Apr 2001  
 GI For diagram(s), see printed CA Issue.  
 AB cf. CA 57, 15107e. 7,9-Dimethyl- and 1,7,9-trimethyl-N,S-purinium betaines were prepared by the conversion of OH, SH, or PhCH<sub>2</sub>S groups in 7,9-dimethyl- and 1,7,9-trimethylpurinium salts, resp., into the SH group and subsequent liberation from the resulting salts. Hypoxanthine (1.5 g.) in 15 g. p-MeC<sub>6</sub>H<sub>4</sub>-SO<sub>3</sub>Me (I) stirred 15 min. at 250° and diluted with 25 cc. BuOH and then 150 cc. Et<sub>2</sub>O yielded 2.3 g. 6-hydroxy-7,9-dimethylpurinium p-toluenesulfonate (II), m. 255-6° (BuOH). II (3.36 g.) and 80 cc. POCl<sub>3</sub> refluxed 2 hrs. and evaporated, treated with 125 cc. absolute EtOH and 7 g. CS(NH<sub>2</sub>)<sub>2</sub> (III), refluxed 2 hrs., cooled, diluted with 400 cc. MeOH, and saturated with dry NH<sub>3</sub> yielded 1.14 g. pale yellow IV (R = H) (V), m. 283° (decomposition from 265° with sintering). 2-NH<sub>2</sub> derivative (3 g.) of II and 150 cc. POCl<sub>3</sub> refluxed 4 hrs., evaporated, treated with 200 cc. absolute EtOH and 10 g. III, refluxed 3.5 hrs., and saturated at 30-5° with dry NH<sub>3</sub> yielded 0.375 g. IV (R = NH<sub>2</sub>) (VI), m. 312° (decomposition) with sintering from 295°. 2-MeS derivative (1.91 g.) of II and 60 cc. POCl<sub>3</sub>, 60 cc. EtOH, and 5 g. III yielded similarly 0.81 g. IV (R = MeS) (VII), m. 277° (decomposition) with sintering from 265°. 7,9-Dimethylxanthinium p-toluenesulfonate (VIII), 125 cc. POCl<sub>3</sub>, and 0.38 cc. H<sub>2</sub>O refluxed 3.5 hrs. and then treated with 150 cc. absolute EtOH and 10 g. III followed by NH<sub>3</sub> gave 1.32 g. pale yellow IX (R = H) (X), m. 300°

(decomposition) with sintering from 285°. 1-Me derivative (3.66 g.) of VIII gave similarly 0.64 g. XI (R = Me) (XII), m. 248° (MeOH). 2-Amino-6-mercaptapurine (0.5 g.) and 5 g. I stirred 10 min. at 117°, diluted with an equal volume EtOH, and treated dropwise with dry Et<sub>2</sub>O gave 0.86 g. VII, m. 281°. VII (2.5 g.) added in portions with stirring to Cl in absolute MeOH gave 0.75 g. 2-amino-6-chloro-7,9-dimethylpurinium chloride (XIII), m. 293° (EtOH); picrate, m. 209° (EtOH). XIII (0.5 g.), 80 cc. absolute EtOH, and 0.5 g. III refluxed 4 hrs. yielded 0.32 g. pale yellow-green 6-SH analog (XIV) of XIII, m. 275°. XIV in MeOH treated with dry NH<sub>3</sub> gave VI. 6-Hydroxy-2-thioxodihdropurine (1.68 g.) in 0.4 g. NaOH in 50 cc. H<sub>2</sub>O treated dropwise with stirring at room temperature during 1 hr. with 1.61 g. PhCH<sub>2</sub>-Cl in 20 cc. MeOH and stirred 4 hrs. yielded 1.6 g. 6-hydroxy-2-benzylthiopurine (XV), m. 262-3° (absolute EtOH). XV (0.5 g.) and 5 g. I yielded 0.69 g. 6-hydroxy-2-benzylthio-7,9-dimethylpurinium p-toluenesulfonate (XVI), m. 240° (EtOH). 2,6-Dithioxotetrahydropurine (2.3 g.) in 250 cc. H<sub>2</sub>O and 1.6 g. NaOH treated dropwise during 2 hrs. with 4.6 g. PhCH<sub>2</sub>Br in 20 cc. MeOH and stirred 5 hrs. yielded 3.1 g. 2,6-bis(benzylthio)purine (XVII), m. 196° (absolute EtOH). XVII (2.5 g.) and 20 g. I stirred 10 min. at 170° yielded 2.02 g. 2,6-bis(benzylthio)7,9-dimethylpurinium p-toluenesulfonate (XVIII), m. 170° (absolute EtOH). 2-Benzylthio-6-thioxo-1-methylidihdropurine (3 g.) and 20 g. I stirred 1 hr. at 150°, cooled, and diluted with 20 cc. absolute EtOH and 500 cc. Et<sub>2</sub>O, and the oily precipitate treated in 500 cc. boiling H<sub>2</sub>O with 10 cc. 65% HClO<sub>4</sub> yielded 2.4 g. 2-benzylthio-6-thioxo-1,7,9-trimethylidihdropurinium perchlorate (XIX), m. 177° (absolute EtOH). 2-Amino-6-benzylthiopurine (0.5 g.) and 5 g. I gave similarly after treatment of the product with 65% HClO<sub>4</sub> 0.56 g. 2-amino-6-benzylthio-7,9-dimethylpurinium perchlorate (XX), m. 226° (EtOH). XVI (0.5 g.), 2 g. AlBr<sub>3</sub>, and 60 cc. dry MePh stirred 6 hrs. at 80° gave 0.16 g. XI (R = H) (XXI), m. 297° (H<sub>2</sub>O). XVIII (1 g.), 4.0 g. AlBr<sub>3</sub>, and 100 cc. dry MePh gave similarly 0.34 g. (crude) pale yellow XXII (R = H) (XXIII), m. 283° (decomposition) (H<sub>2</sub>O). XIX (1 g.), 5 g. AlBr<sub>3</sub>, and 150 cc. dry MePh yielded similarly 0.245 g. (crude) yellow XXII (R = Me) (XXIV), m. 255° (decomposition). XX (0.5 g.), 2 g. AlBr<sub>3</sub>, and 60 cc. dry MePh gave 0.24 g. pale yellow 2-amino-6-mercapto-7,9-dimethylpurinium bromide, m. 270° (EtOH); a 0.5-g. portion in 25 cc. MeOH treated with dry NH<sub>3</sub> gave 0.31 g. VI, m. 312°. 6-Oxo-2-thioxo-3-methyltetrahydropurine (4.0 g.) in 250 cc. H<sub>2</sub>O and 2.0 g. NaOH with 4.1 g. PhCH<sub>2</sub>Br yielded 4.6 g. 2-benzylthio-6-oxo-3-methylidihdropurine (XXV), m. 218° (absolute EtOH). XXV (1.0 g.) and 5.0 g. I stirred 45 min. at 150°, and the oily product treated in 100 cc. BuOH with 3 cc. 65% HClO<sub>4</sub> and then 200 cc. Et<sub>2</sub>O yielded 0.56 g. 2-benzylthio-6-oxo-3,7,9-trimethylidihdropurinium perchlorate (XXVI), m. 202° (absolute EtOH). XXVI (1.0 g.), 5.0 g. AlBr<sub>3</sub>, and 150 cc. dry MePh yielded 0.45 g. (crude) 6-oxo-2-thioxo-3,7-dimethyltetrahydropurine, m. 308° (with sintering from 290°) (H<sub>2</sub>O). V (0.200 g.) added in portions to 1 cc. 30% H<sub>2</sub>O<sub>2</sub>, and the sirupy product in 20 cc. MeOH treated successively with 0.5 cc. 30% H<sub>2</sub>O<sub>2</sub> and dry NH<sub>3</sub> gave 0.115 g. 6-hydroxy-7,9-dimethylpurinium betaine (XXVII). Hypoxanthine (1.5 g.) in 15.0 g. I stirred 15 min. at 150° gave 2.3 g. 6-hydroxy-7,9-dimethylpurinium p-toluenesulfonate (XXVIII), m. 255-6° (BuOH). XXVIII (1.5 g.) in 150 cc. hot MeOH treated at room temperature with dry NH<sub>3</sub> gave 0.5 g. XXVII, m. 309°. XXVII (about 100 mg.) in 10-20 cc. MeOH treated with 5-6 drops 65% HClO<sub>4</sub> gave the perchlorate analog of XXVIII, m. 171° with sintering from 130° (BuOH). X.H<sub>2</sub>O (0.400 g.) added in portions at 30° to 2 cc. 30% H<sub>2</sub>O<sub>2</sub> and treated after 2 hrs. with dry NH<sub>3</sub> yielded 0.175 g. 7,9-dimethylxanthinium betaine (XXIX) (perchlorate, m. 281°), which was also obtained similarly from VII, XXI, and XXIII. 2-Hydroxy-6-thioxo-1-methylidihdropurine (3.64 g.) and 6.0 g. I in 25 cc. AcNMe<sub>2</sub> heated 15 min. at 145° gave 4.13 g. (crude) 2-hydroxy-6-thioxo-1,7,9-trimethylidihdropurinium p-toluenesulfonate; a 3.00-g. portion in 150 cc. MeOH treated at room temperature with concentrated NH<sub>4</sub>OH yielded 0.85 g. 2-hydroxy-6-thioxo-1,7,9-trimethylidihdropurinium betaine (XXX), m. 355-7° (decomposition) (H<sub>2</sub>O). The oxidation of XXX with H<sub>2</sub>O<sub>2</sub> gave 1,7,9-trimethylxanthinium betaine (XXXa) which was also obtained from XII and XXIV.

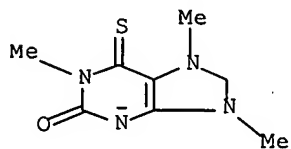
VI oxidized similarly gave 2-amino-6-hydroxy-7,9-dimethylpurinium betaine (XXXI). The R<sub>f</sub> values were determined with 2:1 BuOH-5N AcOH (A), 2:1 PrOH-H<sub>2</sub>O (B), 5% aqueous NH<sub>4</sub>Cl (C), and 4% aqueous Na citrate (D), and the pK<sub>a</sub> values in H<sub>2</sub>O at 20° were measured potentiometrically or spectroscopically for the compds. listed in the table. The uv spectra of X, XII, XXI, XXIII, XXIV,XXX are recorded. Compound, A, B, C, D, pK<sub>a</sub>; V, 0.40, 0.60, 0.81, 0.80, 5.56 ± 0.04; VI, 0.41, 0.51, 0.66, 0.71, 6.28 ± 0.03; VII, 0.62, 0.75, 0.74, 0.66, 4.74 ± 0.08; X, 0.32, 0.50, 0.70, 0.65, 1.9 ± 0.2; XXX, 0.58, 0.72, 0.69, 0.66, 2.1 ± 0.2; XXI, 0.25, 0.41, 0.77, 0.73, 1.85 ± 0.2; XII, 0.42, 0.63, 0.79, 0.76, 1.95 ± 0.2; XXIII, 0.38, 0.57, 0.63, 0.58, 0.83 ± 0.13; XXIV, 0.57, 0.75, 0.57, 0.55, 0.71 ± 0.04; XXVII, 0.28, 0.50, 0.58, 0.87, --; XXXI, 0.30, 0.46, 0.81, 0.84, --; XXIX, 0.21, 0.38, 0.85, 0.76, --; XXXa, 0.40, 0.58, 0.90, 0.84, --; .

IT 5752-14-7P, Purinium compounds, 1,6-dihydro-2-hydroxy-7,9-dimethyl-6-thioxo-, hydroxide, inner salt 5752-18-1P, Purinium, 1,6-dihydro-2-hydroxy-1,7,9-trimethyl-6-thioxo-, hydroxide, inner salt 5752-62-5P, Purinium, 1,6-dihydro-2-mercapto-7,9-dimethyl-6-oxo-, hydroxide, inner salt 5752-63-6P, Purinium, 1,6-dihydro-2-mercapto-7,9-dimethyl-6-thioxo-, hydroxide, inner salt 5752-64-7P, Purinium, 1,6-dihydro-2-mercapto-1,7,9-trimethyl-6-thioxo-, hydroxide, inner salt 5992-44-9P, Purinium, 1,6-dihydro-2-mercapto-1,7,9-trimethyl-6-oxo-, hydroxide, inner salt  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 5752-14-7 CAPLUS  
 CN Purinium, 1,6-dihydro-2-hydroxy-7,9-dimethyl-6-thioxo-, hydroxide, inner salt (8CI) (CA INDEX NAME)



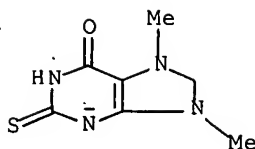
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 5752-18-1 CAPLUS  
 CN Purinium, 1,6-dihydro-2-hydroxy-1,7,9-trimethyl-6-thioxo-, hydroxide, inner salt (8CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

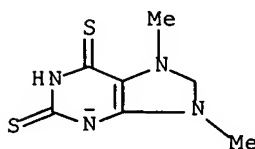
RN 5752-62-5 CAPLUS  
 CN Purinium, 1,6-dihydro-2-mercapto-7,9-dimethyl-6-oxo-, hydroxide, inner salt (8CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 5752-63-6 CAPLUS

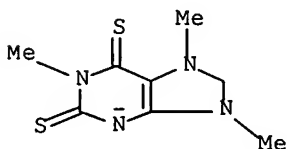
CN Purinium, 1,6-dihydro-2-mercapto-7,9-dimethyl-6-thioxo-, hydroxide, inner salt (8CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 5752-64-7 CAPLUS

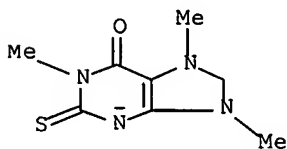
CN Purinium, 1,6-dihydro-2-mercapto-1,7,9-trimethyl-6-thioxo-, hydroxide, inner salt (8CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 5992-44-9 CAPLUS

CN Purinium, 1,6-dihydro-2-mercapto-1,7,9-trimethyl-6-oxo-, hydroxide, inner salt (8CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L57 ANSWER 88 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

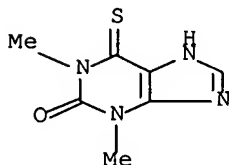
ACCESSION NUMBER: 1966:11492 CAPLUS Full-text

DOCUMENT NUMBER: 64:11492

ORIGINAL REFERENCE NO.: 64:2087a-d

TITLE: Demethylation of 3-methyl-6-methylthiopurines with hydrogen sulfide

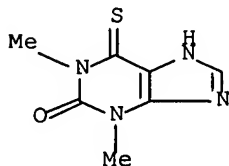
AUTHOR(S): Neiman, Z.; Bergmann, F.  
 CORPORATE SOURCE: Hebrew Univ.-Hadassah Med. School, Jerusalem  
 SOURCE: Israel J. Chem. (1965), 3(3), 85-9  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 22 Apr 2001  
 GI For diagram(s), see printed CA Issue.  
 AB The title compds., with the quinonoid form of the imidazole ring, readily undergo thiohydrolysis in aqueous solution (I, R = H), (II, R = H), (VII), , (VIII); (III, R = Me), (IV, R = Me), , , ; (V, R = Ph), (VI, R = Ph), , , . Thus, H<sub>2</sub>S bubbled during 20 min. at room temperature through a suspension of I in 25% NH<sub>4</sub>OH and the solution evaporated to dryness in vacuo gives 70% II. Similarly, III gives 60% IV, decomposed 300° (AcOH); V in Me<sub>2</sub>NCHO containing 0.1 volume N NaOH gives VI, decomposed 280-5° (dilute AcOH); and VII gives 80% VIII. 6-Methylthiopurine (non-quinonoid imidazole ring) is unchanged under the same conditions. A mixture of 22 g. 8-phenylhypoxanthine, 100 g. P<sub>2</sub>S<sub>5</sub>, and 500 ml. dry β-picoline was stirred and refluxed 4 hrs., the solvent removed in vacuo, the residue treated 1 hr. with 200 ml. H<sub>2</sub>O at 70°, the insoluble material triturated with 2N NaOH, and the mixture filtered through Celitè. The solution was decolorized with C, acidified with AcOH, the precipitate dissolved in 5% Na<sub>2</sub>CO<sub>3</sub>, the solution heated with C, filtered, and cooled. The Na salt which separated was dissolved in hot H<sub>2</sub>O and hot saturated aqueous NH<sub>4</sub>Cl added to give 80% yellow needles of 6-mercapto-8-phenylpurine (IX), decomposed 300°. A solution of 39 g. IX in 600 ml. Me<sub>2</sub>NCHO containing 75 ml. MeI was refluxed 2 hrs., 40 ml. MeI added, reflux continued 2 hrs., and the mixture cooled. The yellow precipitate was dissolved in H<sub>2</sub>O and the pH adjusted to 10 with 2N NaOH to yield 48% V, m. 196-8° (iso-PrOH). Similarly, 6-mercapto-8-methylpurine gave 47% III, m. 195° (MeCN). A solution of 2.5 g. 6-thiotheophylline (VIII) in 15 ml. N NaOH stirred 4 hrs. at room temperature with 2.5 ml. MeI, neutralized with AcOH, evaporated to dryness in vacuo, and the residue extracted with iso-PrOH gave 22% VII, m. 189-91° (iso-PrOH). Uv and chromatographic data are given.  
 IT 2398-70-1, Theophylline, 6-thio-  
 (spectrum of)  
 RN 2398-70-1 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 89 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1965:400859 CAPLUS Full-text  
 DOCUMENT NUMBER: 63:859  
 ORIGINAL REFERENCE NO.: 63:129g-h  
 TITLE: Mass spectrum of thiotheophylline  
 AUTHOR(S): Chaigneau, Marcel; Valdener, Georges; Seyden-Penne, Jacqueline  
 CORPORATE SOURCE: C.N.R.S., Paris  
 SOURCE: Compt. Rend. (1965), 260(14 (Groupe 8)), 3965-8



DOCUMENT TYPE: Journal  
 LANGUAGE: French  
 ED Entered STN: 22 Apr 2001  
 AB The mass spectrum has a relatively very intense mol. peak, and several other peaks which are explained by fragmentation and rearrangement processes. The analogy with the fragmentation mode of theophylline is striking.  
 IT 2398-70-1, Theophylline, 6-thio-  
     (mass spectrum of)  
 RN 2398-70-1 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 90 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1964:425465 CAPLUS Full-text  
 DOCUMENT NUMBER: 61:25465  
 ORIGINAL REFERENCE NO.: 61:4377g-h,4378a  
 TITLE: Purine derivatives  
 INVENTOR(S): Hitchings, George H.; Elion, Gertrude B.  
 PATENT ASSIGNEE(S): Burroughs Wellcome & Co. (U.S.A.) Inc.  
 SOURCE: 2 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3135754		19640602	US 1962-215774	19620809 <--
PRIORITY APPLN. INFO.:			US	19620809 <--

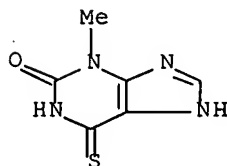
ED Entered STN: 22 Apr 2001  
 AB Continuation-in-part of U.S. 3,056,785 (CA 58, 5701e). These new compds., useful when used in combination with p-aminobenzoic acid antagonists, strongly inhibited *Proteus vulgaris* (strain 49210 I), and were active against transplantable rodent tumors such as Adenocarcinoma 755. A solution of 25 g. 6-iodopurine (I) and 16.8 g. 6-mercaptopyrimidine hydrate in 100 ml. 2N NaOH steam bath heated 24 hrs., was cooled and neutralized with AcOH. The yellow precipitate of 22 g. 6,6-dipurinyl sulfide dihydrate (II) was collected, washed with H<sub>2</sub>O, and dried in vacuo. A mixture of 2.5 g. I, 1.12 g. 4-mercaptopyrimidine, and 10 ml. 2N NaOH yielded 6-(4-pyrimidinyl)thiopurine (III), m. 184-5° (decomposition). A mixture of 7.3 g. 6-thioguanine, 10 g. I, and 60 ml. 2N NaOH yielded 6-(2-amino-6-purinyl)thiopurine (IV), not melting above 325°. A mixture of 10 g. I, 5.12 g. 4-thiouracil, and 60 ml. 2N NaOH yielded 6-(2-hydroxy-4-pyrimidinyl)thiopurine (V). The ultraviolet absorption spectrum showed maximum  $\lambda$  275 and 308 m $\mu$  at pH 1, and 285 and 312 m $\mu$  at pH 11 for II; at 273 and 300 m $\mu$  at pH 1, and 280 and 305 m $\mu$  at pH 11 for III; at 270, 302, and 330 m $\mu$  at pH 1, and 287 and 328 m $\mu$  at pH 11 for IV; and at 320 m $\mu$  at pH 1, and 310 m $\mu$  at pH 11 for V.  
 IT 33285-76-6P, Purin-2(3H)-one, 6-mercapto-3-methyl-

RL: PREP (Preparation)

(preparation of)

RN 33285-76-6 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 91 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1964:425464 CAPLUS Full-text

DOCUMENT NUMBER: 61:25464

ORIGINAL REFERENCE NO.: 61:4377e-g

TITLE: Alkylthiopurines

INVENTOR(S): Hitchings, George H.; Elion, Gertrude B.

PATENT ASSIGNEE(S): Burroughs Wellcome &amp; Co. (U.S.A.) Inc.

SOURCE: 2 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3135753		19640602	US 1961-108986	19610510 <--
PRIORITY APPLN. INFO.:			US	19610510 <--

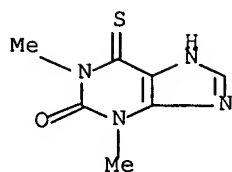
ED Entered STN: 22 Apr 2001

AB The title compds. possess a much improved coronary flow index, 4 and 5, compared to 1 for aminophylline, and are useful in relieving the symptoms angina pectoris. A mixture of 4.3 g. 3-methylhypoxanthine, 12 g. powdered P2S5, and 100 ml. dry pyridine (I) was refluxed 2.5 hrs., I removed in vacuo, and the solid residue heated with 200 ml. H2O for 20 min. to give 3.25 g. 3-methyl-6-purinethione (II), m. of 322-3° (decomposition). A mixture of 10 g. 1,3-dimethylxanthine (III), 50 g. powdered P2S5, and 150 ml. Tetralin heated 5 hrs. at 190° yielded 5.2 g. 2,6-dithiotheophylline, m. 252-4° (decomposition). A mixture of 5 g. III, 15 g. P2S5, and 150 ml. I refluxed 2 hrs. yielded 3.5 g. crude 6-thiotheophylline, m. 315-17° (decomposition). A mixture of 1 g. 3-methylxanthine, 5 g. P2S5, and 50 ml. I refluxed 3 hrs. yielded 0.7 g. 3-methyl-2-oxo-6-mercaptopurine, decompose 320°. A mixture of 5.6 g. 3-methyl-2-thioxanthine, 20 g. P2S5, and 250 ml. I refluxed yielded 3.2 g. 3-methyl-2,6-dithioxanthine, m. >340°. The ultraviolet absorption spectra of these compds. were given. Cf. CA 50, 1933c.

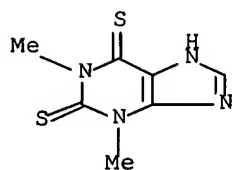
IT 2398-70-1P, Theophylline, 6-thio- 6501-94-6P, Theophylline, dithio- 33285-76-6P, Purin-2(3H)-one, 6-mercapto-3-methyl- 33285-77-7P, Xanthine, 3-methyl-2,6-dithio-  
 RL: PREP (Preparation)  
 (preparation of)

RN 2398-70-1 CAPLUS

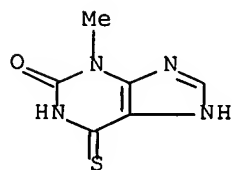
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



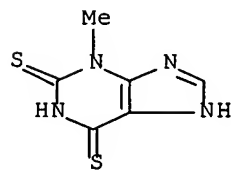
RN 6501-94-6 CAPLUS  
 CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



RN 33285-76-6 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 33285-77-7 CAPLUS  
 CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)



L57 ANSWER 92 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1964:84708 CAPLUS Full-text  
 DOCUMENT NUMBER: 60:84708  
 ORIGINAL REFERENCE NO.: 60:14874c-e  
 TITLE: Action of 8-azaguanine and 8-azaxanthine on  
 Pseudomonas aeruginosa  
 AUTHOR(S): Bergmann, F.; Ungar-Waron, Hanna; Kwietny-Govrin,

Hanna  
 CORPORATE SOURCE: Hebrew Univ.-Hadassah Med. School  
 SOURCE: (1964), 91(2), 270-6  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

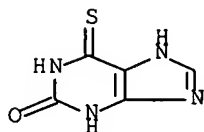
ED Entered STN: 22 Apr 2001

AB 8-Azaguanine does not inhibit the growth of *P. aeruginosa*, but undergoes slow deamination. 8-Azaxanthine arrests the growth of this species temporarily. This growth retardation is abolished by hypoxanthine, xanthine, and a number of unnatural purines. During growth inhibition by azaxanthine, the xanthine oxidase-like activity of the bacterial cells is enhanced. Much larger increments of enzymic activity are obtained by the addition of hypoxanthine, xanthine, or certain unnatural purines, which all contain an unsubstituted imidazole ring. During growth inhibition by 8-azaxanthine, the urate oxidase-like activity of the bacteria is strongly depressed. On the other hand, the addition of hypoxanthine or xanthine to the culture medium produces a huge increase in the enzymic activity of the normal strain. After the 1st exposure to 8-azaxanthine a resistant strain emerges. This strain shows normal xanthine oxidase and urate oxidase activities, even when growing in the presence of the antimetabolite. Benzimidazole and benzotriazole are weak growth inhibitors. They depress xanthine oxidase activity of the bacterial cells, but leave their urate oxidase activity unaffected.

IT 2002-59-7, Xanthine, 6-thio- 2487-40-3, Xanthine,  
 2-thio- 28139-02-8, Xanthine, 3-methyl-2-thio-  
 (effect on *Pseudomonas aeruginosa* response to 8-azaxanthine)

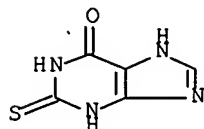
RN 2002-59-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



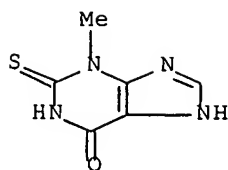
RN 2487-40-3 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



RN 28139-02-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 93 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1964:60225 CAPLUS Full-text

DOCUMENT NUMBER: 60:60225

ORIGINAL REFERENCE NO.: 60:10497a-b

TITLE: Kinetic studies on the methylation of thiopurines

AUTHOR(S): Bergmann, F.; Kleiner, M.

CORPORATE SOURCE: Hebrew Univ.-Hadassah Med. School, Jerusalem

SOURCE: Israel J. Chem. (1963), 1, 477-82

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

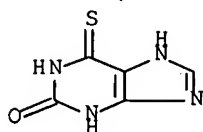
ED Entered STN: 22 Apr 2001

AB Reaction of 6-mercaptapurine (I) with MeI in HCONMe<sub>2</sub> was followed by paper chromatography and ultraviolet spectra; in a 2 step process, viz., alkylation at the S atom, followed by alkylation at N3, it gave 3-methyl-6-methylthiopurine. 6-Thioxanthine (II) underwent a similar 2 step methylation. Comparison of kinetics of the 2 systems (i.e. with I and II) and the exceedingly fast rate of S-methylation of 3-methyl-6-purinethione (III) showed that I reacted through a tautomeric form having a quinonoid structure in the pyrimidine ring. A similar fixed quinonoid structure in III explained its fast methylation. The S-Me group had no marked influence on alkylation at N3.

IT 2002-59-7, Xanthine, 6-thio- 33285-76-6, Xanthine,  
3-methyl-6-thio-  
(methylation of)

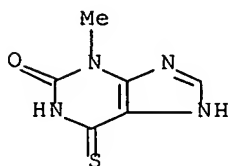
RN 2002-59-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



RN 33285-76-6 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 94 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1964:9768 CAPLUS Full-text  
 DOCUMENT NUMBER: 60:9768  
 ORIGINAL REFERENCE NO.: 60:1748a-d  
 TITLE: Direct thiation of pyrimidinol derivatives  
 AUTHOR(S): Ueda, Takeo; Tsuji, Tadakazu; Momona, Hiroko  
 CORPORATE SOURCE: Keio-Gijuku Univ., Tokyo  
 SOURCE: Chemical & Pharmaceutical Bulletin (1963),  
 11(7), 912-17  
 CODEN: CPBTAL; ISSN: 0009-2363  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 OTHER SOURCE(S): CASREACT 60:9768

ED Entered STN: 22 Apr 2001

GI For diagram(s), see printed CA Issue.

AB 2-Methyl-6-amino-4-pyrimidinethiol, yellow, m. 298° (decomposition); 6-amino-2,4-pyrimidinedithiol, yellow, m. 309° (decomposition); and 2-methyl-5,6-diamino-4-pyrimidinethiol, brownish-yellow, m. 28,5° (decomposition) were prepared in 40 to 50% yield by refluxing 0.005 mol of the appropriate amino-4-pyrimidinol and 0.0125 mol P2S5 in 20 mL. Et3N or 3-picoline for 1 to 15 h. After concentration in vacuo the residue was poured into H2O, made basic with NaOH, filtered hot, neutralized with AcOH, chilled, and the precipitated product recrystd. from H2O. The appropriate 5-acylamino-6-amino-4-pyrimidinols (I) refluxed 8 h. with P2S5 in pyridine, the solvent removed in vacuo, the residue dissolved in H2O, kept 12 h., warmed 1 h. on a water bath, made basic, and chilled, gave II (R1, R2, R3, m.p., and % yield given): NH2, NH2, Me, 248-50°, 81.1; Me, NH2, Me, 192-4°, 81.5. Adjusting the filtrate to pH 5.6 gave III (R1, R2, R3, m.p., % yield given): Me, SH, Me, >300°, 12.2; SH, OH, Me, >300°, 89; SH, SH, Me, >300°, 86.9; Me, SH, H, -, -; Me, SH, OH, (from I, R3 = OEt), >300°, -. Similarly, III (R1 = NH2, R2 = OH, R3 = Et), reacts with P2S5 in pyridine to form III (R1 = NH2, R2 = SH, R3 = Et), orange-yellow, m. >300°. None of these compds. shows significant activity against poliomyelitis virus.

IT 91184-09-7P, Xanthine, 8-methyl-2-thio- 91184-18-8P,

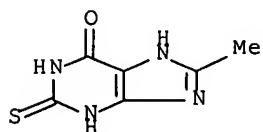
Xanthine, 8-methyl-2,6-dithio-

RL: PREP (Preparation)

(preparation of)

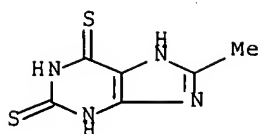
RN 91184-09-7 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-8-methyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 91184-18-8 CAPLUS

CN Xanthine, 8-methyl-2,6-dithio- (7CI) (CA INDEX NAME)



L57 ANSWER 95 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1963:60954 CAPLUS Full-text

DOCUMENT NUMBER: 58:60954

ORIGINAL REFERENCE NO.: 58:10464a-e

TITLE: Relation of structure to the inhibitory activity of purines against urate oxidases

AUTHOR(S): Bergmann, F.; Kwietny-Govrin, Hanna; Ungar-Waron, Hanna; Kalmus, A.; Tamari, M.

CORPORATE SOURCE: Hebrew Univ.-Hadassah Med. School, Jerusalem

SOURCE: Biochemical Journal (1963), 86, 567-74

CODEN: BIJOAK; ISSN: 0264-6021

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

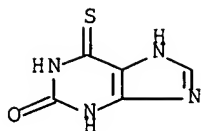
ED Entered STN: 22 Apr 2001

AB cf. *ibid.* 292. The inhibitory activity of a variety of compds. against urate oxidase has been determined: 150 values in  $\mu\text{M}$  were for hypoxanthine 220, 8-hydroxy-purine 110, 2-hydroxypurine 12, 2,8-dihydroxypurine 5.2, xanthine 18, 6,8-dihydroxypurine 66, 6-mercaptopurine 700, 6-thioxanthine 2.7, 2-thioxanthine 190, 8-hydroxy-6-mercaptopurine 70, 6-hydroxy-8-mercaptopurine 500, 6,8-dimercaptopurine 370, 8-hydroxy-2-mercaptopurine 500, 2-hydroxy-8-mercaptopurine 12, 2-thiouric acid 250, 6-thiouric acid 14, 8-thiouric acid 5, 2,6-dithiouric acid 150, 2,8-dithiouric acid 80, 6,8-dithiouric acid 0.4, 6,8-dihydroxy-2-methylmercaptopurine 500, 2,6-dihydroxy-8-methylmercaptopurine 38, 2-hydroxy-6-methylmercaptopurine 6, 8-hydroxy-6-methylmercaptopurine 32, 2,8-dihydroxy-6-methylmercaptopurine 0.1, 3, 8-hydroxy-3-methyl-6-methylmercapto-2-oxopurine 7, 4,5-diamino-6-thiouracil 38, 2,4-dihydroxypteridine 300, 2,4,6-trihydroxypteridine 150, 2,4,6,7-tetrahydroxypteridine 500, 8-aza-6-hydroxypurine 47, 8-aza-2-hydroxypurine 1.6, 8-azaxanthine 5.9, 3-methyl-2-thiouric acid 150, 3-methyl-6-thiouric acid 400, 3-methyl-8-thiouric acid 190, 3-methyl-2-thioxanthine 100, 3-methyl-6-thioxanthine 100, 7-methyl-6-thioxanthine 1000. The inhibitory effect was used to measure the affinity of the inhibitors for the enzyme. Of the 3 O atoms of uric acid, that of the 2-carbonyl group possesses the greatest binding power for the active center. Replacement of this O atom by S greatly diminishes the inhibitory activity. Combination of a 2-carbonyl group with S at C-6 enhances inhibitory activity considerably. On certain purine derivs., a 6-methylmercapto substituent is more effective than a 6-thiocarbonyl group. 2,6-Dihydroxy-6-methylmercaptopurine is the most potent inhibitor of urate oxidase known so far. Replacement of the imidazole moiety of the purine ring by triazole enhances affinity, whereas introduction of the pyrazine ring, as in pteridines, greatly decreases it. Free imino groups are essential for the attachment of purines to urate oxidase, as N-methylation weakens or abolishes the inhibitory effect. On the other hand, in 2-thiopurines, methylation at N-3 increases the inhibitory power.

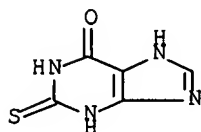
IT 2002-59-7, Xanthine, 6-thio- 2487-40-3, Xanthine, 2-thio- 28139-02-8, Xanthine, 3-methyl-2-thio- 33285-76-6, Xanthine, 3-methyl-6-thio- (uric oxidase inhibition by)

RN 2002-59-7 CAPLUS

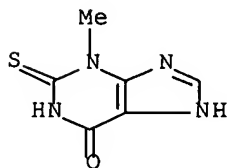
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



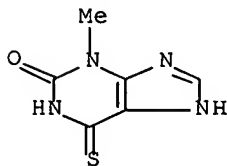
RN 2487-40-3 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



RN 28139-02-8 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



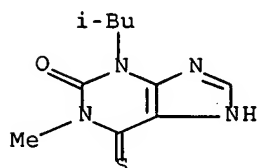
RN 33285-76-6 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 96 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1963:48836 CAPLUS Full-text  
 DOCUMENT NUMBER: 58:48836  
 ORIGINAL REFERENCE NO.: 58:8327a-b  
 TITLE: Observations concerning the effects of a thioxanthine upon the heart of the intact animal  
 AUTHOR(S): Maxwell, G. M.; Elliott, R. B.; Kneebone, G. M.



CORPORATE SOURCE: Univ. Adelaide  
 SOURCE: Australian J. Exp. Biol. Med. Sci. (1962),  
 40, 335-40  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 ED Entered STN: 22 Apr 2001  
 AB An intravenous dose of 1.0 mg. 3-isobutyl-1-methyl-6-thioxanthine/kg.  
 administered to dogs gave statistically significant increases in respiratory  
 rate, respiratory volume, O consumption, CO2 production, and pulse rate.  
 Femoral and pulmonary arterial pressures decreased as did the calculated total  
 peripheral resistance. Coronary blood flow and cardiac metabolic rates for O  
 and CO2 increased. Cardiac efficiency and coronary vascular resistance  
 decreased.  
 IT 42458-91-3, Xanthine, 3-isobutyl-1-methyl-6-thio-  
 (heart response to)  
 RN 42458-91-3 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo-  
 (9CI) (CA INDEX NAME)



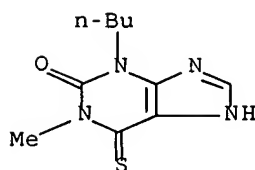
L57 ANSWER 97 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1963:20789 CAPLUS Full-text  
 DOCUMENT NUMBER: 58:20789  
 ORIGINAL REFERENCE NO.: 58:3445a-b  
 TITLE: 3-Butyl-1-methyl-6-thioxanthine  
 PATENT ASSIGNEE(S): May & Baker Ltd.  
 SOURCE: 3 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR M188		19610320	FR	19600812 <--
PRIORITY APPLN. INFO.:			FR	19600812 <--

OTHER SOURCE(S): MARPAT 58:20789

ED Entered STN: 22 Apr 2001  
 AB The title compound can be used in compns. which dilate bronchial tubes. PS5  
 (56 g.) is added to 33 g. 3-butyl-1-methylxanthine and 500 ml. anhydrous  
 pyridine, the mixture refluxed 8 hrs., cooled, 1000 ml. H2O added carefully,  
 the mixture evaporated in vacuo, the precipitate filtered off, washed with  
 H2O, dissolved in 300 ml. 0.8N NaOH, and the solution acidified with HOAc to  
 give 35 g. 1-methyl-3-butyl-6-thioxanthine, m. 156-8°.  
 IT 42458-90-2P, Xanthine, 3-butyl-1-methyl-6-thio-  
 RL: PREP (Preparation)  
 (manufacture of)  
 RN 42458-90-2 CAPLUS  
 CN 2H-Purin-2-one, 3-butyl-1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA

INDEX NAME)



L57 ANSWER 98 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1962:436343 CAPLUS Full-text

DOCUMENT NUMBER: 57:36343

ORIGINAL REFERENCE NO.: 57:7262i, 7263a-e

TITLE: Preparation and properties of 1,2-dihydrophthalazine derivatives

AUTHOR(S): Smith, Richard F.; Otremba, Edward D.

CORPORATE SOURCE: State Univ. Coll., Albany, NY

SOURCE: Journal of Organic Chemistry (1962), 27, 879-82

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

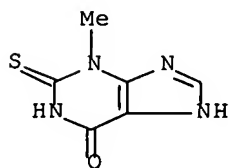
OTHER SOURCE(S): CASREACT 57:36343

ED Entered STN: 22 Apr 2001

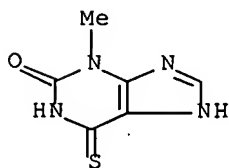
AB cf. CA 53:17143d. Reduction of 2-methyl-and 2-ethylphthalazinium iodide (I, II) with aqueous NaBH<sub>4</sub> yielded the corresponding 2-alkyl-1,2-dihydrophthalazines (III, IV). H<sub>2</sub>O (3 l.) containing 0.3 mole o-HO<sub>2</sub>CC<sub>2</sub>H<sub>4</sub>CHO stirred at 80° with 0.3 mole (N<sub>2</sub>H<sub>4</sub>)<sub>2</sub>.H<sub>2</sub>SO<sub>4</sub> and 1 l. 1.1 N NaOH, the green suspension evaporated in vacuo to 200 ml., extracted with C<sub>6</sub>H<sub>6</sub>, and the dried (MgSO<sub>4</sub>) exts. evapd, yielded 50% phthalazine (V), m. 87-90°. Further extraction of the aqueous solution with EtOAc gave 0.9 g. 1(2H)-phthalazinone, m. 183-4°. I, m. 240-3° (decomposition), heated with saturated alc. picric acid (20 ml./g, halide) gave 75% picrate, m. 199-200° (decomposition). II, m. 225-8° (decomposition) (alc.), similarly yielded 93% II picrate, m. 167-9°. V (2 g.) and 4 ml. PhCH<sub>2</sub>Cl refluxed 3 hrs. in 15 ml. dry MeOH, the cooled mixture diluted with anhydrous Et<sub>2</sub>O, kept overnight, and the Et<sub>2</sub>O-washed product dried in vacuo yielded 89% extremely hygroscopic 2-benzylphthalazinium chloride (VI), m. 175-8° (alc.-Et<sub>2</sub>O); picrate m. 183-4° (MeOH). The powdered quaternary salts added portionwise to 3% aqueous NaBH<sub>4</sub> (3:1 salt-hydride), the cooled mixture extracted with Et<sub>2</sub>O, the extract dried (MgSO<sub>4</sub>), and the product isolated gave 2-alkyl-1,2-di-hydrophthalazines. Distillation yielded 75% III, b<sub>17</sub> 129-30°; HCl salt m. 133-5° (decomposition) (alc.); pierate m. 95-8° (decomposition); MeI salt (VII) m. 173-6° (MeOH). III on exposure to air rapidly yielded 2-methyl-1(2H)-phthalazi-none, m. 108-10°. IV HCl salt, m. 142-4° (decomposition) (alc.), converted to the free base, refluxed 6 hrs. with excess MeI in ale., the resultant highly decompd, tarry product extracted with EtOAc and the extract diluted with Et<sub>2</sub>O gave IV MeI salt, m. 155-7° (alc.). VI (4.0 g.) reduced with aqueous NaBH<sub>4</sub>, the oily product refluxed 3 hrs. with 7 ml. MeI in 25 ml. alc., and the mixture cooled gave 1.4 g. VII. Dilution of the filtrate c with Et<sub>2</sub>O gave 1.4 g. unidentified material, m. 138-42°, recrystd. from alc.-Et<sub>2</sub>O to give a sample, m. 140-2° (decomposition), melting with evolution of a potent lacrimator. VII (1 g.) in 10 ml. H<sub>2</sub>O treated with 10 ml. 6N NaOH and the oily product extracted with Et<sub>2</sub>O gve o-Me<sub>2</sub>NCH<sub>2</sub>C<sub>4</sub>CN; picrate m. 144-5°; MeI salt m. 184-5°; HCl salt m. 226-7° (alc), v 2220 cm.<sup>-1</sup>, identical with the salt prepd, by stirring 0.05 mole each 0-

BrCH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>CN, Me<sub>2</sub>NH.HCl, and anhydrous Na<sub>2</sub>CO<sub>3</sub> 2 days at 20° in 50 ml. MeOH, acidifying the coned, solution with dilute HCl, basifying the Et<sub>2</sub>O-washed aqueous layer, extracting with Et<sub>2</sub>O, and treating the dried extract with anhydrous HCl.

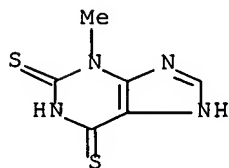
IT 28139-02-8P, Xanthine, 3-methyl-2-thio- 33285-76-6P,  
Xanthine, 3-methyl-6-thio- 33285-77-7P, Xanthine,  
3-methyl-2,6-dithio- 38695-85-1P, Xanthine, 1-methyl-6-thio-  
91184-08-6P, Xanthine, 1-methyl-2-thio- 91184-17-7P,  
Xanthine, 1-methyl-2,6-dithio-  
RL: PREP (Preparation)  
(preparation of)  
RN 28139-02-8 CAPLUS  
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX  
NAME)



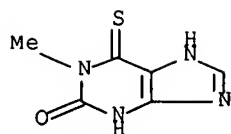
RN 33285-76-6 CAPLUS  
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX  
NAME)



RN 33285-77-7 CAPLUS  
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)

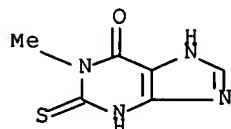


RN 38695-85-1 CAPLUS  
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX  
NAME)



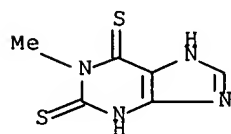
RN 91184-08-6 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1-methyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 91184-17-7 CAPLUS

CN Xanthine, 1-methyl-2,6-dithio- (7CI) (CA INDEX NAME)



L57 ANSWER 99 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1962:436342 CAPLUS Full-text

DOCUMENT NUMBER: 57:36342

ORIGINAL REFERENCE NO.: 57:7262h-i

TITLE: Condensed pyrimidine systems. XXII. N-methyl purines

AUTHOR(S): Elion, Gertrude B.

CORPORATE SOURCE: Burroughs Wellcome and Co. Inc., Tuckahoe, NY

SOURCE: Journal of Organic Chemistry (1962), 27, 2478-91

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 57:36342

ED Entered STN: 22 Apr 2001

AB cf. CA 54, 18531b. A group of 1-and 3-monomethylpurines has been prepared by complete synthesis. Among the new derivs. are 3-methyladenine, 3-methylguanine, and the 1-and 3-methyl derivatives of 6-mercaptapurine. A number of 7- and 9-methyl derivs. have been obtained by direct methylation of 6-chloropurine, conversion to the mercapto derivs., and subsequent separation of the 7- and 9-methylpurine-6-thiols. Several ring openings and rearrangements have been observed in the course of attempts to prepare 1-methyladenine.

IT 28139-02-8P, Xanthine, 3-methyl-2-thio- 33285-76-6P, Xanthine, 3-methyl-6-thio- 33285-77-7P, Xanthine, 3-methyl-2,6-dithio- 38695-85-1P, Xanthine, 1-methyl-6-thio-

91184-08-6P, Xanthine, 1-methyl-2-thio- 91184-17-7P,

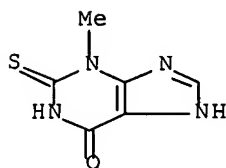
Xanthine, 1-methyl-2,6-dithio-

RL: PREP (Preparation)

(preparation of)

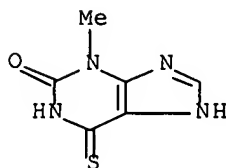
RN 28139-02-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



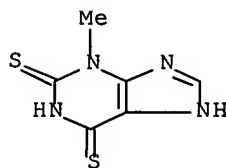
RN 33285-76-6 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



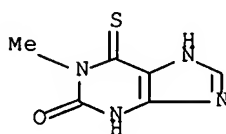
RN 33285-77-7 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)



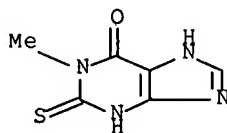
RN 38695-85-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



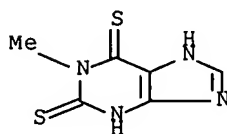
RN 91184-08-6 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1-methyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 91184-17-7 CAPLUS

CN Xanthine, 1-methyl-2,6-dithio- (7CI) (CA INDEX NAME)



L57 ANSWER 100 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1962:429662 CAPLUS Full-text

DOCUMENT NUMBER: 57:29662

ORIGINAL REFERENCE NO.: 57:5924h-i,5925a-i,5926a-b

TITLE: The synthesis of some 6-thioxanthines

AUTHOR(S): Wooldridge, K. R. H.; Slack, R.

CORPORATE SOURCE: May Baker Ltd., Dagenham, UK

SOURCE: Journal of the Chemical Society (1962)  
1863-28

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 57:29662

ED Entered STN: 22 Apr 2001

AB A series of 1,3- and 3,7-disubstituted 6-thioxanthines, of interest as broncho and coronary dilators, has been prepared by the selective thionation of the corresponding xanthines with P2S5 in C5H5N. 1,3,7-Trialkyl-6- thioxanthines could not be prepared in this way but were readily obtained from 1,3-dialkyl-6-thioxanthines. Theophylline (50 g.), 100 g. P2S3, and 1. dry C5H5N refluxed 8 hrs. with stirring, cooled, diluted with stirring during 1 hr. with 2 l. H2O, concentrated to about 1/3 volume, cooled, and filtered, and the residue dissolved in 2N NaOH, filtered, and reprecipitated with dilute HCl yielded 51 g. 1,3-dimethyl-6-thioxanthine (I), pale yellow needles, m. 323-5° (decomposition) (EtOH or H2O). 6-Thiotheobromine (75 g.) with 150 g. P2S5 gave similarly 72 g. 3,7-dimethyl-6-thioxanthine (II), m. 300-1°. (MeNH)2CS (79 g.) added in portions with stirring during 0.5 hr. to 65 g. NCCH2CO2H in 156 g. Ac2O and 200 cc. AcOH at 65°, kept 2 hrs. at 65° evaporated at 69-5° in vacuo, and the gummy residue stirred at 50° with 200 cc. H2O and adjusted to pH 10 with 50% aqueous NaOH gave 65 g. 6-amino-1,3-dimethyl 2-thiouracil (III), prisms, m. 286-8° (EtOH). The crude III suspended in 6000 cc. H2O containing 25.5 g. NaNO2 at 80-90°, 50 cc. AcOH added during 15 min., and the mixture stirred 15 min. at 80-90° and cooled yielded crude 5-NO derivative (IV) of III, blue-green amorphous solid, m. 215-16° (decomposition). The IV added in 5-g.

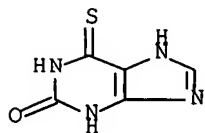
portions to 2.5 l. H<sub>2</sub>O at 70-80° together with sufficient Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub> to discharge the color of the IV, cooled, and filtered, the residual 5-NH<sub>2</sub> derivative of III, m. 230-4°, added immediately to 500 cc. 2N H<sub>2</sub>SO<sub>4</sub>, the resulting sulfate (57 g.) boiled 0.5 hr. with 500 cc. HCONH<sub>2</sub>, diluted with 250 cc. H<sub>2</sub>O, and cooled, and the yellow solid dissolved in 300 cc. hot 17% NH<sub>4</sub>OH, filtered, and acidified to pH 4 with AcOH yielded 47 g. 1,3-dimethyl-2-thioxanthine, m. 344-8°. Me<sub>2</sub>SO<sub>4</sub> (25.2 g.) added dropwise in 15 min. with stirring at 40° to 35 g. I and 100 cc. 2N NaOH, kept 0.5 hr. at 40°, cooled, and filtered gave 15 g. 1,3,7-trimethyl-6-thioxanthine (V), pale yellow prisms, m. 246-7°. II (17.5 g.) and 42.5 g. Me<sub>2</sub>SO<sub>4</sub> gave 1 g. V, m. 247-9°. II (10g.) in 125 cc. 0.5N NaOH stirred 2 hrs. at room temperature with 10.7 g. MeI yielded 6.7 g. 1,2,3,4-tetrahydro-3,7-dimethyl-1-methylthiopurine, needles, m. 300-3° (H<sub>2</sub>O). The appropriate urea was converted by the method of Traube [Ber. 33, 3035(1900)] or of Speer and Raymond (CA 48, 1346h) or of Montgomery (CA 50, 13932b) to the corresponding 1,3-dialkylxanthines (1- and 3-alkyl group and m.p. given): Me, MeO(CH<sub>2</sub>)<sub>3</sub>, 166-8°; Me, furfuryl, 255-8°; Et, iso-Bu, 195-7°; Pr, iso-Bu, 189-92°; Bu, Me, 207-10°. Similarly were prepared 3-isobutylxanthine (VI), m. 299-301°, and the 7-Me derivative of VII, m. 239-41°. P<sub>2</sub>S<sub>5</sub> (600 g.) and 482 g. 3-isobutyl-1-methylxanthine in 4.2 l. dry C<sub>5</sub>H<sub>5</sub>N, refluxed 9 hrs. with stirring, cooled to about 40°, diluted carefully with H<sub>2</sub>O, concentrated to about 2.5 l., diluted with 3.5 l. H<sub>2</sub>O, and filtered, and the residue dissolved in 2.5 l. warm N NaOH, filtered, and acidified with concentrated HCl to pH 4 pp.d. 426 g. 3-isobutyl-1-methyl-6-thioxanthine (VII), yellow prisms, m. 170-2° (EtOH). Similarly were prepared the following 1,3-disubstituted-6-thioxanthines (1- and 3-substituent, m.p., and % yield given): Me, Me (VIII), 3235°, 94; Me, Et, 235-7°, 79; Me, Pr, 164-7°, 63; Me, Bu, 156-8°, 73; Me, Am, 169-70°, 50; Me, C<sub>6</sub>H<sub>13</sub>, 167-74°, 78; Me, iso-Am, 156-60°, 50; Me, MeO(CH<sub>2</sub>)<sub>3</sub>, 150-2°, 50; Me, CH<sub>2</sub>:CHCH<sub>2</sub>, 152-6°, 81; Me, CH:CMech<sub>2</sub>, 195-8°, 47; Me, PhCH<sub>2</sub>, 213-15°, 84; Me, Ph(CH<sub>2</sub>)<sub>2</sub>, 198-9°, 63; Me, furfuryl, 184-6°, 15; Et, Me, 235-9°, 76; Et, Et, 2568°, 72; Et, Bu, 175-8°, 74; Et, iso-Bu, 180-3°, 39; Et, CH<sub>2</sub>:CHCH<sub>2</sub>, 210-12°, 49; Pr, Pr, 212-15°, 89; Bu, Me, 295-8°, 84; Bu, Bu, 183-6°, 72. Similarly were prepared the following 8-substituted VIII (substituent, m.p., and % yield given): Me, 294-5°, 75; Et, 218-19°, 76; SH, 240° (decomposition), 83. I (42 g.) and 8.6 g. NaOH in 150 cc. H<sub>2</sub>O stirred 0.5 hr. at room temperature, cooled, and filtered, and the dried Na salt (44 g.) of I dissolved in 200 cc. HCONMe<sub>2</sub>, treated with stirring during 15 min. at room temperature with 18.6 g. AcCH<sub>2</sub>Cl, stirred 0.5 hr., diluted with 300 cc. iced H<sub>2</sub>O, and filtered gave 21.3 g. 7-AcCH<sub>2</sub> derivative (IX) of I, yellow needles, m. 208-10°. IX (21 g.), 269 g. paraformaldehyde, 11.9 g. piperidine-HCl, 1.6 cc. Et<sub>2</sub>O.BF<sub>3</sub>, and 200 cc. dry dioxane stirred 7 hrs. at 100° and filtered gave 23.0 g. 1,3-dimethyl-7(2-oxo-4-piperidinobutyl)-6-thioxanthine-HCl, yellow-brown prisms, m. 197-200°. In the same manner as VII were prepared the following 1,3,7-trisubstituted-6-thioxanthines (1-, 3-, and 7-substituents and m.p. given): Me, Me, Et, 22830°; Me, Me, Et<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>, 52-4°; Me, iso-Bu, Et<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub> [isolated as the (-)-di(p-toluoyl) D-tartrate], 120° (decomposition); Me, iso-Bu, AcCH<sub>2</sub>, 170-4°; Bu, Me, Me, 118-19°. In the same manner were prepared the following 3,7-dialkyl-6thioxanthines (3- and 7-substituents and m.p. given): Me, Me, 300-1°; Bu, Me, 200-3°; iso-Bu, Me, 228-30°. Also prepared was 3-methyl-6-thioxanthine, m. 269-74°. Choline chloride (3.4 g.) in 900 cc. hot iso-PrOH treated with stirring with 150 g. 85% KOH in 600 cc. absolute MeOH, cooled to 0°, filtered, treated with 500 g. VII, warmed a few min., and evaporated in vacuo, the residual sirup dissolved in 1 l. hot isoPrOH, treated with C, filtered, diluted with 1 l. dry Et<sub>2</sub>O, and cooled, and the precipitated filtered off gave 548 g. choline salt of VII, pale yellow prisms, m. 145-9°; their mother liquor evaporated, and the sirupy residue dissolved in H<sub>2</sub>O and acidified to pH 4 with HCl gave 8 g. VII. Similarly were prepared the choline salts of the following 1,3-disubstituted-6-thioxanthines (1- and 3-substituents, m.p. and % yield given): Me, Me (X), 145-7°, 47; Me, Et, 157-9°, 72; Me, Pr, 145-50°, 72; Me, Bu, 133-5°, 88; Me, Am, 150-3°, 93; Me, C<sub>6</sub>H<sub>13</sub>, 55-7°, 94; Me, iso-Bu, 148.5-

9.5°, 92; Me, iso-Am, 125-8°, 90; Me, CH<sub>2</sub>:CHCH<sub>2</sub>, 172-5°, 73; Me, CH<sub>2</sub>:CMeCH<sub>2</sub>, 145-51°, 80; Me, PhCH<sub>2</sub>, 166-71°, 80; Me, Ph(CH<sub>2</sub>)<sub>2</sub>, 173-5°, 80; Et, Me, 157-8°, 70; Et, Et, 142-7°, 92; Et, Bu, 115-18°, 79; Pr, Pr, 114-18°, 57; Bu, Me, 105-9°, 62. Also prepared were 8-Me derivative of X, 175-6°, 65, and the 8-SH derivative of X, 209 11°, 70. The ultraviolet absorption maximum of a number of thioxanthines are tabulated.

IT 2002-59-7, Xanthine, 6-thio-  
(derivs.)

RN 2002-59-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



IT 2398-70-1P, Theophylline, 6-thio- 6603-63-0P,  
Theophylline, 2-thio- 40915-18-2P, Xanthine, 1,3-dibutyl-6-thio-  
42458-87-7P, Xanthine, 3-ethyl-1-methyl-6-thio-  
42458-88-8P, Xanthine, 1-methyl-3-propyl-6-thio-  
42458-90-2P, Xanthine, 3-butyl-1-methyl-6-thio-  
42458-91-3P, Xanthine, 3-isobutyl-1-methyl-6-thio-  
42458-92-4P, Xanthine, 1-methyl-3-(2-methylallyl)-6-thio-  
42458-93-5P, Xanthine, 1-methyl-3-pentyl-6-thio-  
42458-94-6P, Xanthine, 3-(3-methoxypropyl)-1-methyl-6-thio-  
42458-95-7P, Xanthine, 3-isopentyl-1-methyl-6-thio-  
42458-96-8P, Xanthine, 3-hexyl-1-methyl-6-thio-  
42458-97-9P, Xanthine, 3-benzyl-1-methyl-6-thio-  
42458-98-0P, Xanthine, 1-methyl-3-phenethyl-6-thio-  
42458-99-1P, Xanthine, 3-furfuryl-1-methyl-6-thio-  
42459-00-7P, Xanthine, 1-ethyl-3-methyl-6-thio-  
42459-01-8P, Xanthine, 1,3-diethyl-6-thio- 42459-02-9P,  
Xanthine, 3-allyl-1-ethyl-6-thio- 42459-03-0P, Xanthine,  
3-butyl-1-ethyl-6-thio- 42459-04-1P, Xanthine,  
1-ethyl-3-isobutyl-6-thio- 42459-06-3P, Xanthine,  
1,3-dipropyl-6-thio- 42459-07-4P, Xanthine, 1-butyl-3-methyl-6-  
thio- 42459-09-6P, Xanthine, 1,3,8-trimethyl-6-thio-  
42459-10-9P, Theophylline, 8-ethyl-6-thio- 90230-11-8P,  
Choline, compound with 6-thiotheophylline 93263-24-2P, Xanthine,  
3-isobutyl-6-thio- 96536-20-8P, Choline, compound with  
3-ethyl-1-methyl-6-thioxanthine 96536-21-9P, Choline, compound  
with 1,3,8-trimethyl-6-thioxanthine 96652-89-0P, Choline, compound  
with 1-ethyl-3-methyl-6-thioxanthine 96986-49-1P, Xanthine,  
1,3-diethyl-6-thio-, compound with choline 97212-72-1P, Choline,  
compound with 1-methyl-3-propyl-6-thioxanthine 97282-72-9P,  
Choline, compound with 3-allyl-1-methyl-6-thioxanthine 97406-00-3P  
, Choline, compound with 3-isobutyl-1-methyl-6-thioxanthine  
97406-02-5P, Choline, compound with 3-butyl-1-methyl-6-thioxanthine  
97439-87-7P, Xanthine, 1-butyl-3-methyl-6-thio-, compound with  
choline 97616-67-6P, Choline, compound with 3-butyl-1-ethyl-6-  
thioxanthine 97767-38-9P, Xanthine, 1-methyl-3-pentyl-6-thio-,  
compound with choline 97767-40-3P, Choline, compound with  
1,3-dipropyl-6-thioxanthine 97783-97-6P, Choline, compound with  
3-isopentyl-1-methyl-6-thioxanthine 98174-21-1P, Choline, compound  
with 3-hexyl-1-methyl-6-thioxanthine 98801-33-3P, Choline,  
compound with 3-benzyl-1-methyl-6-thioxanthine 99688-81-0P,

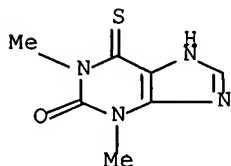


Choline, compound with 1-methyl-3-phenethyl-6-thioxanthine  
 106802-46-4P, Choline, compound with 1-methyl-3-(2-methylallyl)-6-  
 thioxanthine 878790-85-3P, Xanthine, 1,3,8-trimethyl-6-thio-,  
 compound with choline 878790-86-4P, Xanthine, 1-ethyl-3-methyl-6-  
 thio-, compound with choline 878790-87-5P, Xanthine,  
 1,3-dipropyl-6-thio-, compound with choline 878794-41-3P,  
 Theophylline, 6-thio-, compound with choline 879632-11-8P,  
 Xanthine, 3-allyl-1-ethyl-6-thio-, compound with choline  
 RL: PREP (Preparation)

(preparation of)

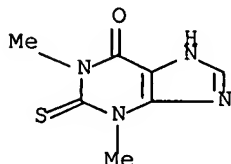
RN 2398-70-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX  
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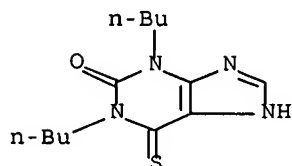
RN 6603-63-0 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX  
 NAME)



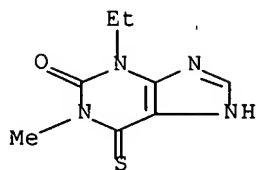
RN 40915-18-2 CAPLUS

CN 2H-Purin-2-one, 1,3-dibutyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX  
 NAME)



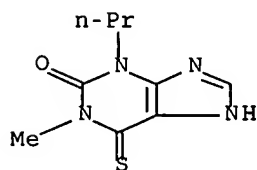
RN 42458-87-7 CAPLUS

CN 2H-Purin-2-one, 3-ethyl-1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA  
 INDEX NAME)



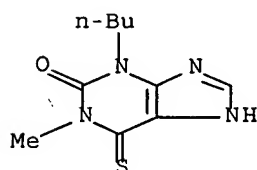
RN 42458-88-8 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



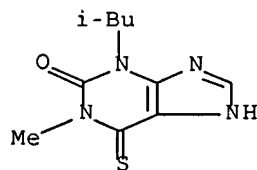
RN 42458-90-2 CAPLUS

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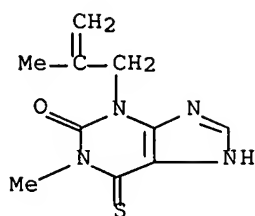
RN 42458-91-3 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



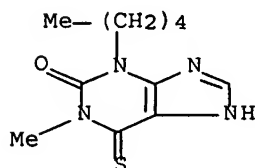
RN 42458-92-4 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methyl-2-propenyl)-6-thioxo- (9CI) (CA INDEX NAME)



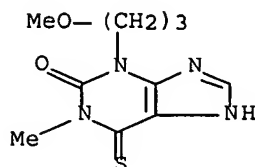
RN 42458-93-5 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-pentyl-6-thioxo- (9CI) (CA INDEX NAME)



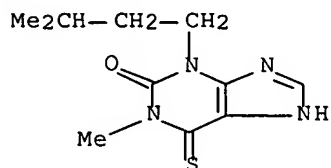
RN 42458-94-6 CAPLUS

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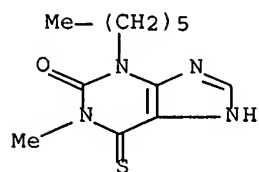
RN 42458-95-7 CAPLUS

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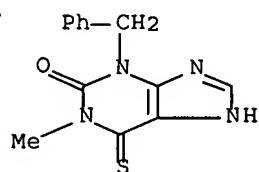
RN 42458-96-8 CAPLUS

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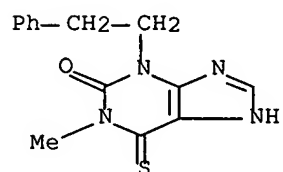
RN 42458-97-9 CAPLUS

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(9CI) (CA INDEX NAME)



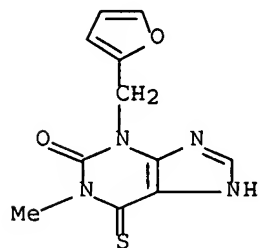
RN 42458-98-0 CAPLUS

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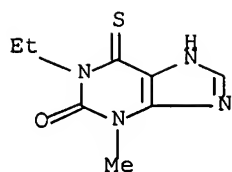
RN 42458-99-1 CAPLUS

CN 2H-Purin-2-one, 3-(2-furanylmethyl)-1,3,6,7-tetrahydro-1-methyl-6-thioxo-  
(9CI) (CA INDEX NAME)



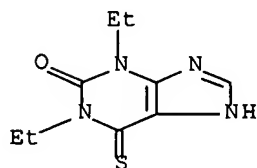
RN 42459-00-7 CAPLUS

CN 2H-Purin-2-one, 1-ethyl-1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA  
INDEX NAME)



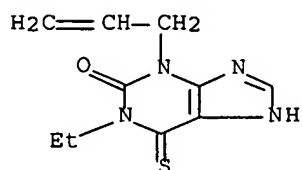
RN 42459-01-8 CAPLUS

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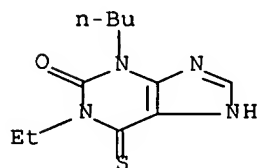
RN 42459-02-9 CAPLUS

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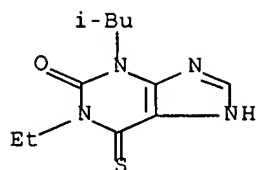
RN 42459-03-0 CAPLUS

CN 2H-Purin-2-one, 3-butyl-1-ethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



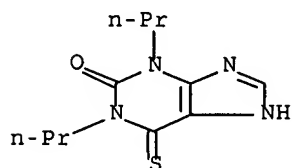
RN 42459-04-1 CAPLUS

CN 2H-Purin-2-one, 1-ethyl-1,3,6,7-tetrahydro-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



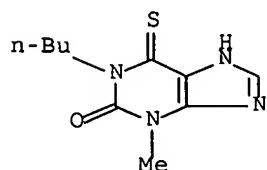
RN 42459-06-3 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dipropyl-6-thioxo- (9CI) (CA INDEX NAME)



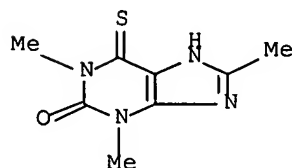
RN 42459-07-4 CAPLUS

CN 2H-Purin-2-one, 1-butyl-1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



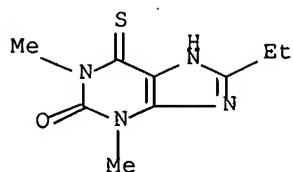
RN 42459-09-6 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3,8-trimethyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 42459-10-9 CAPLUS

CN 2H-Purin-2-one, 8-ethyl-1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



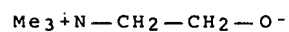
RN 90230-11-8 CAPLUS

CN Choline, compd. with 6-thiotheophylline (6CI, 7CI) (CA INDEX NAME)

CM 1

CRN 44519-34-8

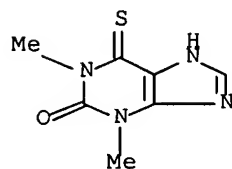
CMF C5 H13 N O



CM 2

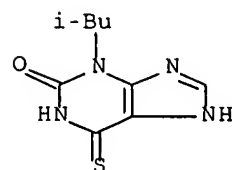
CRN 2398-70-1

CMF C7 H8 N4 O S



RN 93263-24-2 CAPLUS

CN Xanthine, 3-isobutyl-6-thio- (7CI) (CA INDEX NAME)



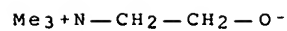
RN 96536-20-8 CAPLUS

CN Choline, compd. with 3-ethyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 44519-34-8

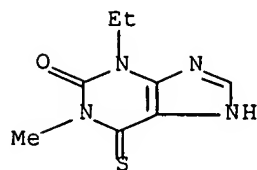
CMF C5 H13 N O



CM 2

CRN 42458-87-7

CMF C8 H10 N4 O S



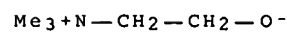
RN 96536-21-9 CAPLUS

CN Choline, compd. with 1,3,8-trimethyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 44519-34-8

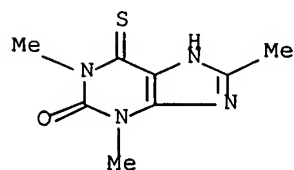
CMF C5 H13 N O



CM 2

CRN 42459-09-6

CMF C8 H10 N4 O S



RN 96652-89-0 CAPLUS

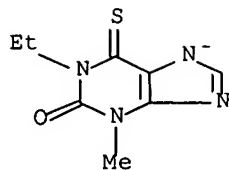
CN Choline, compd. with 1-ethyl-3-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 96652-88-9

CMF C8 H9 N4 O S

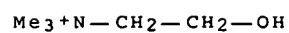




CM 2

CRN 62-49-7

CMF C5 H14 N O



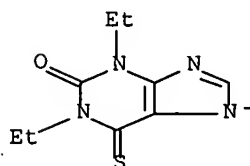
RN 96986-49-1 CAPLUS

CN Choline, compd. with 1,3-diethyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 96986-48-0

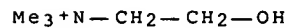
CMF C9 H11 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O



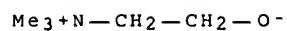
RN 97212-72-1 CAPLUS

CN Choline, compd. with 1-methyl-3-propyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 44519-34-8

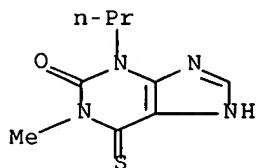
CMF C5 H13 N O



CM 2

CRN 42458-88-8

CMF C9 H12 N4 O S



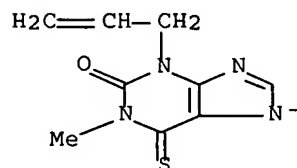
RN 97282-72-9 CAPLUS

CN Choline, compd. with 3-allyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 97282-71-8

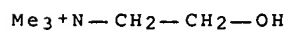
CMF C9 H9 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O



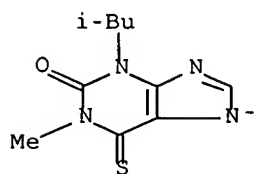
RN 97406-00-3 CAPLUS

CN Choline, compd. with 3-isobutyl-1-methyl-6-thioxanthine (6CI, 7CI) (CA INDEX NAME)

CM 1

CRN 97405-99-7

CMF C10 H13 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O

 $\text{Me}_3\text{N}-\text{CH}_2-\text{CH}_2-\text{OH}$ 

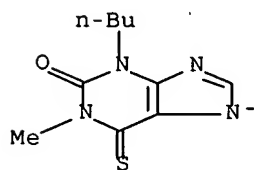
RN 97406-02-5 CAPLUS

CN Choline, compd. with 3-butyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 97406-01-4

CMF C10 H13 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O

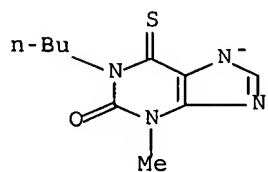
 $\text{Me}_3\text{N}-\text{CH}_2-\text{CH}_2-\text{OH}$ 

RN 97439-87-7 CAPLUS

CN Choline, compd. with 1-butyl-3-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

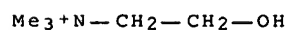
CM 1

CRN 97439-86-6  
CMF C10 H13 N4 O S



CM 2

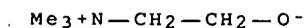
CRN 62-49-7  
CMF C5 H14 N O



RN 97616-67-6 CAPLUS  
CN Choline, compd. with 3-butyl-1-ethyl-6-thioxanthine (7CI) (CA INDEX NAME)

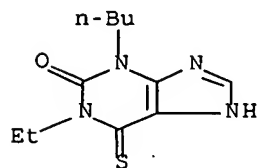
CM 1

CRN 44519-34-8  
CMF C5 H13 N O



CM 2

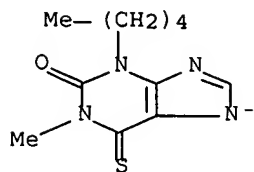
CRN 42459-03-0  
CMF C11 H16 N4 O S



RN 97767-38-9 CAPLUS  
CN Choline, compd. with 1-methyl-3-pentyl-6-thioxanthine (7CI) (CA INDEX NAME)

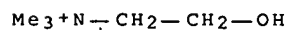
CM 1

CRN 97767-37-8  
CMF C11 H15 N4 O S



CM 2

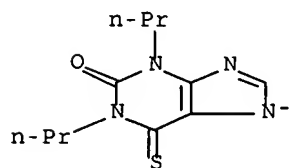
CRN 62-49-7  
CMF C5 H14 N O



RN 97767-40-3 CAPLUS  
CN Choline, compd. with 1,3-dipropyl-6-thioxanthine (7CI) (CA INDEX NAME)

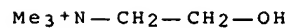
CM 1

CRN 97767-39-0  
CMF C11 H15 N4 O S



CM 2

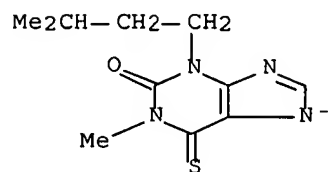
CRN 62-49-7  
CMF C5 H14 N O



RN 97783-97-6 CAPLUS  
CN Choline, compd. with 3-isopentyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

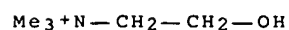
CM 1

CRN 97783-96-5  
CMF C11 H15 N4 O S



CM 2

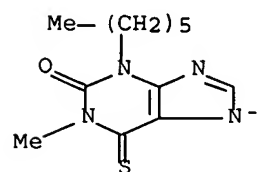
CRN 62-49-7  
CMF C5 H14 N O



RN 98174-21-1 CAPLUS  
CN Choline, compd. with 3-hexyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

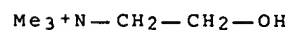
CM 1

CRN 98174-20-0  
CMF C12 H17 N4 O S



CM 2

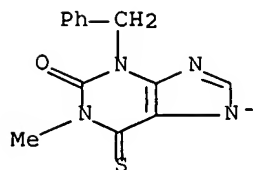
CRN 62-49-7  
CMF C5 H14 N O



RN 98801-33-3 CAPLUS  
CN Choline, compd. with 3-benzyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

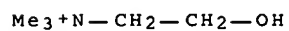
CM 1

CRN 98801-32-2  
CMF C13 H11 N4 O S



CM 2

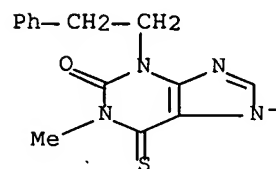
CRN 62-49-7  
CMF C5 H14 N O



RN 99688-81-0 CAPLUS  
CN Choline, compd. with 1-methyl-3-phenethyl-6-thioxanthine (7CI) (CA INDEX NAME)

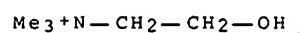
CM 1

CRN 99688-80-9  
CMF C14 H13 N4 O S



CM 2

CRN 62-49-7  
CMF C5 H14 N O

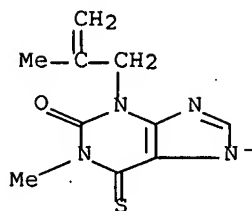


RN 106802-46-4 CAPLUS  
CN Choline, compd. with 1-methyl-3-(2-methylallyl)-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 106802-45-3

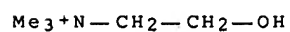
CMF C10 H11 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O



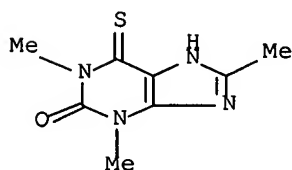
RN 878790-85-3 CAPLUS

CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1,3,6,7-tetrahydro-1,3,8-trimethyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 42459-09-6

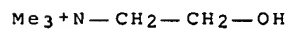
CMF C8 H10 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O



RN 878790-86-4 CAPLUS

CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1-ethyl-1,3,6,7-

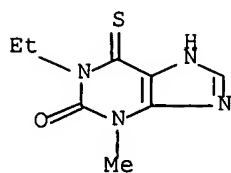


tetrahydro-3-methyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 42459-00-7

CMF C8 H10 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O

$\text{Me}_3\text{N}-\text{CH}_2-\text{CH}_2-\text{OH}$

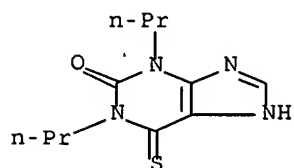
RN 878790-87-5 CAPLUS

CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1,3,6,7-tetrahydro-1,3-dipropyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 42459-06-3

CMF C11 H16 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O

$\text{Me}_3\text{N}-\text{CH}_2-\text{CH}_2-\text{OH}$

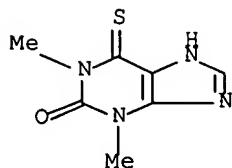
RN 878794-41-3 CAPLUS

CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 2398-70-1

CMF C7 H8 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O

$\text{Me}_3\text{N}-\text{CH}_2-\text{CH}_2-\text{OH}$

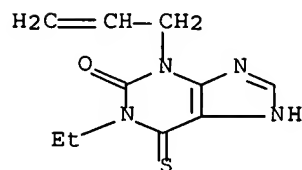
RN 879632-11-8 CAPLUS

CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1-ethyl-1,3,6,7-tetrahydro-3-(2-propenyl)-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 42459-02-9

CMF C10 H12 N4 O S



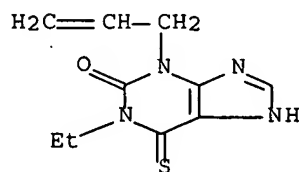
CM 2

CRN 62-49-7

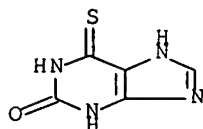
CMF C5 H14 N O

$\text{Me}_3\text{N}-\text{CH}_2-\text{CH}_2-\text{OH}$

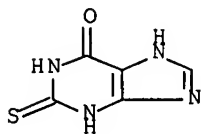
IT 42459-02-9, Xanthine, 3-allyl-1-ethyl-6-thio-  
 (sodium derivative, blood-vessel and bronchial dilation by)  
 RN 42459-02-9 CAPLUS  
 CN 2H-Purin-2-one, 1-ethyl-1,3,6,7-tetrahydro-3-(2-propenyl)-6-thioxo- (9CI)  
 (CA INDEX NAME)



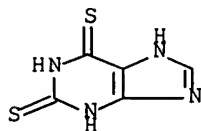
L57 ANSWER 101 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1962:418827 CAPLUS Full-text  
 DOCUMENT NUMBER: 57:18827  
 ORIGINAL REFERENCE NO.: 57:3862h-i,3863a  
 TITLE: Specific reactions of the purine-oxidizing system of  
 Pseudomonas aeruginosa  
 AUTHOR(S): Bergmann, Felix; UngarWaron, Hanna; Kwietny-Govrin,  
 Hanna; Goldberg, Hilda; Leon, Shalom  
 CORPORATE SOURCE: Hebrew Univ., Jerusalem, Israel  
 SOURCE: Biochimica et Biophysica Acta, Specialized Section on  
 Nucleic Acids and Related Subjects (1962),  
 55, 512-22  
 CODEN: BBASB7; ISSN: 0926-6550  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 22 Apr 2001  
 AB cf. CA 55, 26059g. Resting cells of -P. aeruginosa oxidized 2-aminopurine and  
 its MeNH- and Me2N- analogs at C-8 in contrast to the action of mammalian  
 xanthine oxidase. 6-Mercaptopurine was attacked 1st at C-2, then at C-8, and  
 then further. This compound did not inhibit growing P. aeruginosa, but  
 increased production of xanthine oxidase. The 3-Me derivs. of thioxanthines  
 were oxidized at C-8, while 3methylhypoxanthine was first attacked at C-2.  
 The resulting complex, containing 3-methylxanthine, dissociated before further  
 oxidation to 3-methyluric acid, in contrast to xanthine. The results are  
 discussed in reference to the mechanism of attack and the different actions of  
 bacterial and mammalian xanthine oxidases. 21 references.  
 IT 2002-59-7, Xanthine, 6-thio- 2487-40-3, Xanthine,  
 2-thio- 5437-25-2, Xanthine, dithio- 28139-02-8,  
 Xanthine, 3-methyl-2-thio- 33285-76-6, Xanthine,  
 3-methyl-6-thio- 33285-77-7, Xanthine, 3-methyl-2,6-dithio-  
 (oxidation by xanthine oxidase of Pseudomonas aeruginosa)  
 RN 2002-59-7 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



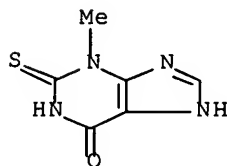
RN 2487-40-3 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



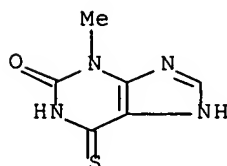
RN 5437-25-2 CAPLUS  
 CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



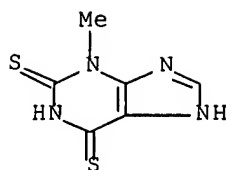
RN 28139-02-8 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 33285-76-6 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 33285-77-7 CAPLUS  
 CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)



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ACCESSION NUMBER: 1962:410979 CAPLUS Full-text

DOCUMENT NUMBER: 57:10979

ORIGINAL REFERENCE NO.: 57:2268g-i,2269a-i,2270a-c

TITLE: Alkaloids of *Tylophora crebriflora*-structure and synthesis of tylocrebrine, a new phenanthroindolizidine alkaloid

AUTHOR(S): Gellert, E.; Govindachari, T. R.; Lakshmikantham, M. V.; Ragade, I. S.; Rudzats, R.; Viswanathan, N.

CORPORATE SOURCE: Univ. N. S. W., Sydney

SOURCE: Journal of the Chemical Society (1962) 1008-14

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

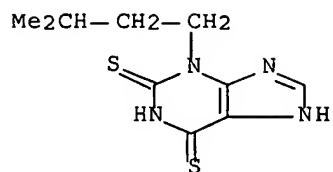
LANGUAGE: Unavailable

ED Entered STN: 22 Apr 2001

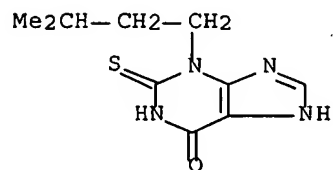
AB Milled *T. crebriflora* (21 lb.) extracted with hot MeOH, the extract concentrated to small volume (4 l.), diluted with 2 l. H<sub>2</sub>O, concd, to 800 ml. in a climbing film evaporator, and the mixture filtered while warm gave a solid (I) and a filtrate (II). II acidified with dilute AcOH, extracted exhaustively with CCl<sub>4</sub>, the combined CCl<sub>4</sub> solns, extracted with 2N HCl, the extract combined with the previous acidic phase, and filtered gave a filtrate (III), which gave a strong Mayer test and showed 2 fluorescent spots when chromatographed on paper in BuOH-AcOH (R<sub>f</sub> 0.2 and 0.5). I in warm 2N AcOH diluted with hot H<sub>2</sub>O, cooled, filtered, the filtrate extracted with CCl<sub>4</sub>, combined with III, made basic with concd, aqueous, the precipitate (45 g.) repeatedly precipitated from hot aqueous AcOH with concd, aqueous NH<sub>3</sub>, extracted (Soxhlet) with MeOH, and the product crystd, from MeOH gave crude alkaloid mixture (IV). Crude IV (in 2 g. batches) subjected to partition chromatography in 15:85 PrOH-2N-AcOH on a cellulose column (partial separation into fractions with R<sub>f</sub> 0.2 and 0.5), the fractions from several such chromatograms combined (intermediate fractions were rechromatographed), the 1st fraction evaporated in vacuo, the residue dissolved in warm dilute AcOH, made alkaline with concd, aqueous NH<sub>3</sub> and the crude alkaloid [R<sub>f</sub> 0.5 (in 3:97 AcOH-BuOH saturated with H<sub>2</sub>O) (solvent A)] crystallized 3 times from MeOH gave tylocrebrine (V), m. 218-20° (decomposition), λ 263, 342, and 360 mμ (ε 4.81, 3.25, and 3.09), [α]<sub>D</sub><sup>24</sup> -45 ± 2° (c 0.74, CHCl<sub>3</sub>), pK<sub>a</sub> 6.7 (in 50% aqueous EtOH) [HI salt m. 214-17° (decomposition) (aqueous MeOH); perchlorate m. 262-4° (decomposition); picrate m. 134-6° (Me<sub>2</sub>CO containing a little MeOH)]. The crude alkaloid [R<sub>f</sub> 0.2 (solvent A)] from the 2nd fraction recrystd. 3 times from CHCl<sub>3</sub>-MeOH gave tylophorine (isomeric with V), m. 282-4° (decomposition), λ 257, 290, 340, 355 mμ (ε 4.82, 4.51, 3.43, 2.96). V refluxed on a H<sub>2</sub>O bath with excess MeI in MeOH until dissolved, then refluxed 30 min. more, concentrated, and cooled gave optically active V.MeI, m. 255-8° (decomposition) (MeOH), [α]<sub>D</sub><sup>21</sup> -30 ± 2° (c 0.30, MeOH). Optically active V.MeI refluxed 30 min. in 20% aqueous NaOH gave (+)-V.MeI, m. 264-6° (decomposition) (MeOH), [α]<sub>D</sub><sup>21</sup> 0° (c 0.10, MeOH). V.MeI (1.4 g.) refluxed with AgCl in aqueous MeOH, the resulting V.MeCl shaken with Ag<sub>2</sub>O in H<sub>2</sub>O, the solution of V.MeOH evaporated to dryness, the residue heated 3 min. at

240°/0.2 mm., and the product chromatographed in C<sub>6</sub>H<sub>6</sub> on basic Al<sub>2</sub>O<sub>3</sub> gave 400 mg. VI, m. 144.5-5.0° (C<sub>6</sub>H<sub>6</sub>-petr. ether, then petr. ether). V.MeI (100 mg.) converted directly into V.MeOH (with Ag<sub>2</sub>O in 10 ml. H<sub>2</sub>O; 5 hr.), the mixture filtered, the filtrate evaporated in vacuo at 50° the residue heated 30 min. at 100°/0.05 mm., the product repeatedly extracted with hot C<sub>6</sub>H<sub>6</sub>, and chromatographed in C<sub>6</sub>H<sub>6</sub> on Al<sub>2</sub>O<sub>3</sub> gave 10 mg. VI, m. 144.5-5.0°. VI (50 mg.) in 3 ml. AcOH heated 5 min. at 125° with excess HIO<sub>4</sub> gave no CH<sub>2</sub>O (no precipitate with dimedon). Et 3,4,6,7-tetramethoxyphenanthrene-9-carboxylate (3 g.) in 25 ml. dry tetrahydrofuran added to 1.5 g. LiAlH<sub>4</sub> in 15 ml. tetrahydrofuran with stirring, stirred 4 hrs., treated with Et<sub>2</sub>O and H<sub>2</sub>O, the organic layer decanted, and evaporated gave 2.2 g. 9 - hydroxymethyl - 3,4,6,7 - tetramethoxyphenanthrene (VII), m. 164-5° (C<sub>6</sub>H<sub>6</sub>). VII (5 g.), 4 ml. SOCl<sub>2</sub>, and 0.5 ml. pyrldine in 120 ml. CHCl<sub>3</sub> heated 15 min. at 40-60°, cooled, poured into H<sub>2</sub>O, extracted with CHCl<sub>3</sub>, the extract dried, concentrated to small volume, and diluted with petr. ether gave 4.2 g. 9-chloromethyl-3,4,6,7-tetramethoxyphenanthrene (VIII), m. 148° (decomposition) (C<sub>6</sub>H<sub>6</sub>-petr. ether). VIII (4 g.) in 40 ml. dry tetrahydrofuran added dropwise with stirring to pyrrolmagnesium bromide (from 1.8 g. Mg, 5.8 ml. EtBr, and 5.26 ml. freshly distilled pyrrole) in Et<sub>2</sub>O cooled in ice under N, stirred 3 hrs. during which the mixture was allowed to reach room temperature, diluted with Et<sub>2</sub>O, decomposed with saturated aqueous NH<sub>4</sub>Cl, the organic layer separated, washed with H<sub>2</sub>O, dried, evaporated, and the residue chromatographed in CHCl<sub>3</sub> on Al<sub>2</sub>O<sub>3</sub> gave 2 g. 2-(3,4,6,7-tetramethoxy-9-phenanthrylmethyl)pyrrole (IX), m. 155-6° (C<sub>6</sub>H<sub>6</sub>-petr. ether). IX (0.4 g.) in 30 ml. AcOH containing 0.25 g. PtO<sub>2</sub> hydrogenated 8 hrs. at room temperature at 60 lb./sq. in., filtered, the filtrate evaporated in vacuo, the residue extracted repeatedly with hot dilute HCl, the combined exts. basified with aqueous NH<sub>3</sub>, and the product isolated with CHCl<sub>3</sub> gave 0.25 g. corresponding pyrrolidine (X), oil; picrate m. 247-9° (AcOH). X (0.5 g.) and 3 ml. 98% HCO<sub>2</sub>H heated 1.5 hrs. at 180°, cooled, dissolved in CHCl<sub>3</sub>, the solution washed, dried, evaporated, the residual N-formyl derivative refluxed 1.5 hrs. with 4 ml. POCl<sub>3</sub> and 15 ml. PhMe, the solution mixture cooled, diluted with petr. ether, the resulting quaternary chloride dried in vacuo, reduced with 0.8 g. NaBH<sub>4</sub> in 30 ml. MeOH, the solution evaporated in vacuo, the residue taken up in CHCl<sub>3</sub>, the solution washed with H<sub>2</sub>O, dried, evaporated, and the residue chromatographed in CHCl<sub>3</sub> on Al<sub>2</sub>O<sub>3</sub> gave 0.2 g. (±)-V, m. 219-21° (CHCl<sub>3</sub>-MeOH). (±)-V (200 mg.) in 10 ml. CHCl<sub>3</sub> refluxed 3 hrs. on a H<sub>2</sub>O bath with 2 ml. MeI and kept overnight at 30°, the solution evaporated, the resulting (±)-V.MeI shaken 5 hrs. with Ag<sub>2</sub>O (from 1 g. AgNO<sub>3</sub>) and 10 ml. H<sub>2</sub>O, and the (±)-V.MeOH subjected to Hofmann degradation as above gave 40 mg. VI, m. 144.5-5.0° (C<sub>6</sub>H<sub>6</sub>-petr. ether). 2-Amino-α-(3,4-dimethoxyphenyl)-4,5-dimethoxycinnamic acid (G. et al., loc. cit.) diazotized in Me<sub>2</sub>CO with BuONO and subjected to Pschorr ring closure gave 2,3,5,6-tetramethoxyphenanthrene-9-carboxylic acid (XI). XI (5 g.) refluxed 4 hrs. with 4 ml. concentrated H<sub>2</sub>SO<sub>4</sub> in 150 ml. MeOH gave 4.2 g. Me ester of XI, m. 150° (EtOH). XI was converted successively as above into 9-hydroxymethyl-2,3,5,6-tetramethoxyphenanthrene, m. 133° (C<sub>6</sub>H<sub>6</sub>); 9-chloromethyl - 2,3,5,6 - tetramethoxyphenanthrene, m. 163-4° (C<sub>6</sub>H<sub>6</sub>-petr. ether); 2-(2,3,5,6-tetramethoxy-9-phenanthrylmethyl)pyrrolidine [picrate m. 218° (decomposition) (AcOH-EtOH)]; and finally 9,11,12,13,13a, 14-hexahydro3,4,6,7-tetramethoxydibenzo [f,h] pyrrolo [1,2-b] isoquinoline (XII), m. 219° (CHCl<sub>3</sub>-MeOH). XII (200 mg.) converted to the methiodide and the product subjected to the Hofmann degradation as above gave 30 mg. XIII, m. 137-8° (C<sub>6</sub>H<sub>6</sub>-petr. ether). The structure of V is shown.

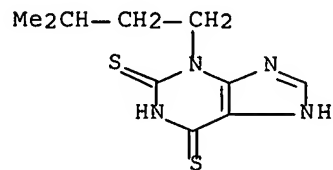
IT 32051-91-5P, Xanthine, 3-isopentyl-2,6-dithio- 94689-49-3P  
 , Xanthine, 3-isopentyl-2-thio-  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 32051-91-5 CAPLUS  
 CN Xanthine, 3-isopentyl-2,6-dithio- (7CI, 8CI) (CA INDEX NAME)



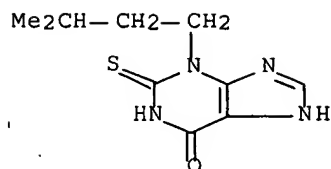
RN 94689-49-3 CAPLUS  
 CN Xanthine, 3-isopentyl-2-thio- (7CI) (CA INDEX NAME)



L57 ANSWER 103 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1962:410978 CAPLUS Full-text  
 DOCUMENT NUMBER: 57:10978  
 ORIGINAL REFERENCE NO.: 57:2268g  
 TITLE: Synthesis of Dihydrotriacanthine  
 AUTHOR(S): Leonard, Nelson J.; Laursen, Richard A.  
 CORPORATE SOURCE: Univ. of Illinois, Urbana  
 SOURCE: Journal of Organic Chemistry (1962), 27,  
 1778-80  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 ED Entered STN: 22 Apr 2001  
 AB 3-Isopentyladenine was synthesized and shown to be identical with  
 dihydrotriacanthine.  
 IT 32051-91-5P, Xanthine, 3-isopentyl-2,6-dithio- 94689-49-3P  
 , Xanthine, 3-isopentyl-2-thio-  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 32051-91-5 CAPLUS  
 CN Xanthine, 3-isopentyl-2,6-dithio- (7CI, 8CI) (CA INDEX NAME)



RN 94689-49-3 CAPLUS  
 CN Xanthine, 3-isopentyl-2-thio- (7CI) (CA INDEX NAME)



L57 ANSWER 104 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1962:410977 CAPLUS Full-text

DOCUMENT NUMBER: 57:10977

ORIGINAL REFERENCE NO.: 57:2267f-i,2268f-g

TITLE: Synthesis of calycotomine and its analogs

AUTHOR(S): Chatterjee, A.; Chaudhury, N. Aditya

CORPORATE SOURCE: Univ. Coll. Sci., Calcutta

SOURCE: Journal of Organic Chemistry (1962), 27, 309-10

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

ED Entered STN: 22 Apr 2001

AB cf. CA 54, 22693g. Liquid NH<sub>3</sub> (300 ml.) containing 8.73 g. Na treated with a thin stream of 22.0 g. 3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> and the mixture kept 6 hrs. with rise of temperature to 30° decompd, by cautious addition of ice and washed twice with 50 ml. Et<sub>2</sub>O, the aqueous phase aerated and the NH<sub>3</sub>-free solo. acidified with AcOH with cooling, washed with Et<sub>2</sub>O and made alkaline with NaHCO<sub>3</sub>, extracted 3 times with 100 ml. BuOH and the dried extract (150 ml.) treated with HCl in Et<sub>2</sub>O yielded 18.0 g. 3,4-HO(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub>.HCl (I), m. 203-4° (absolute alc.Et<sub>2</sub>O). I (0.9 g.) and 0.4 g. HOCH<sub>2</sub>CHO in 10 ml. H<sub>2</sub>O adjusted to pH 4.,5-5.0 and kept 3 days at 30° basified with Na<sub>2</sub>CO<sub>3</sub> and extracted with CHCl<sub>3</sub> gave 0.6 g. 6-demethylcalycotomine (II, R<sub>1</sub> = OH, R<sub>2</sub> = OMe) (III), m. 198-200° (decomposition). III (0.6 g.) in 50 ml. dry Et<sub>2</sub>O added slowly to CH<sub>2</sub>N<sub>2</sub> [from Me(NO)NCONH<sub>2</sub>] and kept 16 hrs. at 28-6° before evapn, in vacuo, the residue (0.5 g.) taken up in 20 ml. 4N HCl and washed 3 times with 25 ml. Et<sub>2</sub>O, the acidic aqueous solution basified with 45 ml. 10% aqueous NaOH and extracted 3 times with 50 ml. CHCl<sub>3</sub> yielded 45-50% dl-calycotomine (II, R<sub>1</sub> = R<sub>2</sub> = OMe), m. 134° (1:1 EtOAc-petr. ether), λ 240, 290 mμ (log ε 3.48, 3.66, alc.); HCl salt m. 195-6° (absolute alc.-Et<sub>2</sub>O). Concentrated HCl (8 ml.) heated 8 hrs. with 5.0 g. 3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> at 160-70° in a sealed tube and the product cooled in an ice bath yielded 4.0 g. 3,4-(HO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>NH<sub>2</sub>HCl (IV), m. 241° (Me<sub>2</sub>CO). IV (1.0 g.) and 0.6 g. HOCH<sub>2</sub>CHO in 10 ml. H<sub>2</sub>O adjusted to pH 3-4 and kept 3 days at 25-6°, concd, in vacuo and the cryst, product recrystd, from 1: 1 alc.-Me<sub>2</sub>CO gave 0.85 g. 6,7-demethylcalycotomine (II, R<sub>1</sub> = R<sub>2</sub> = OH), m. 208-9° (decomposition), λ 288 mμ (log ε 3.57). Condensation of 0.08 g. with 0.15 g. 3,4-(HO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H.HCl in 5 ml. H<sub>2</sub>O at pH 4-5 gave 0.1 g. 3-carboxy-6,7-demethylealycotomine, m. 281-2° (decomposition), λ 280 mμ (log ε 3.54).

IT 32051-91-5P, Xanthine, 3-isopentyl-2,6-dithio- 94689-49-3P

, Xanthine, 3-isopentyl-2-thio-

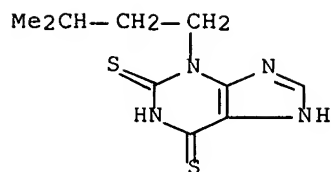
RL: PREP (Preparation)

(preparation of)

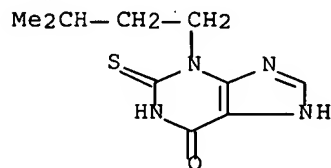
RN 32051-91-5 CAPLUS

CN Xanthine, 3-isopentyl-2,6-dithio- (7CI, 8CI) (CA INDEX NAME)





RN 94689-49-3 CAPLUS  
 CN Xanthine, 3-isopentyl-2-thio- (7CI) (CA INDEX NAME)



L57 ANSWER 105 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1962:66964 CAPLUS  
 DOCUMENT NUMBER: 56:66964  
 ORIGINAL REFERENCE NO.: 56:12912a-c  
 TITLE: N-Alkyl thiopurines  
 PATENT ASSIGNEE(S): Wellcome Foundation Ltd.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 887409		19620117	GB 1958-17890	19580604 <--
PRIORITY APPLN. INFO.:			US	19570606 <--

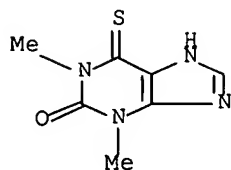
ED Entered STN: 22 Apr 2001

AB The title compds., which increase the flow of blood in coronary vessels, were prepared by treating an N-alkoxypurine with P2S5 at 115-200° in an inert solvent. Thus, 4.3 g. 3-methylhypoxanthine, 12 g. P2O5, and 100 ml. pyridine was refluxed 2.5 hrs., the pyridine removed under reduced pressure, and the residue heated with 200 ml. water 20 min. to give 3-methyl-6-thiohypoxanthine (3.25 g. crude), m. 322-3° (H2O), λ 242, 335 mμ (pH 1) and 242, 333 mμ (pH 11). Theophylline (I) (10 g.), 50 g. P2S5, and 150 ml. tetrahydronaphthalene heated 5 hrs. at 190° gave 1,3-dimethyl-2,6-dithioxanthine (5.2 g.), m. 252-4° (95% alc.), λ 252, 297, 345 mμ (pH 1) and 265, 295, 345 mμ (pH 11). I (5 g.) and 15 g. P2S5 refluxed 2 hrs. in 150 ml. pyridine gave 1,3-dimethyl-6-thioxanthine, m. 315-17° (95% alc.), λ 270, 342 mμ (pH 1) and 260, 340 mμ (pH 11). Similarly prepared were 3-methyl-6-thioxanthine, m. 320°, λ 345 mμ (pH 1) and 337 mμ (pH 11), and 3-methyl-2,6-dithioxanthine, m. 340°, λ 254, 298, 352 mμ (pH 1) and 257, 302, 342 mμ (pH 11).

IT 2398-70-1P, Theophylline, 6-thio- 6501-94-6P,  
 Theophylline, dithio- 33285-76-6P, Xanthine, 3-methyl-6-thio-  
 33285-77-7P, Xanthine, 3-methyl-2,6-dithio-  
 RL: PREP (Preparation)  
 (preparation of)

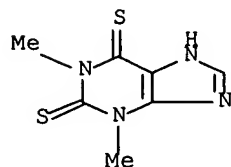
RN 2398-70-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



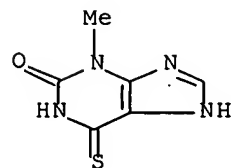
RN 6501-94-6 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



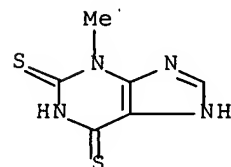
RN 33285-76-6 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 33285-77-7 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)



L57 ANSWER 106 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1962:41798 CAPLUS Full-text

DOCUMENT NUMBER: 56:41798

ORIGINAL REFERENCE NO.: 56:7935c-f  
 TITLE: Structure-activity relations in a series of  
 6-thioxanthines with bronchodilator and coronary  
 dilator properties  
 AUTHOR(S): Armitage, A. K.; Boswood, Janet; Large, B. J.  
 SOURCE: British Journal of Pharmacology and Chemotherapy ( 1961), 17, 196-207  
 CODEN: BJPCAL; ISSN: 0366-0826

DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

ED Entered STN: 22 Apr 2001

AB The bronchodilator, coronary dilator, central stimulant, and diuretic activities of forty-seven 1,3-and 3,7-disubstituted and 1,3,7-trisubstituted 6-thioxanthines are reported. Bronchodilator activity was determined on the isolated guinea pig tracheal ring preps. and coronary dilator activity on the dog heart-lung preps. Diuretic activity was determined using conscious rats, and stimulant activity using mice. The in vivo bronchodilatory activity was determined by the protection afforded to guinea pigs against bronchoconstrictor aerosol. While choline 6-thiotheophyllinate is twice as active as choline theophyllinate as a broncho- and coronary dilator, several higher members of the theophylline series are more active than the 6-thio analogs. The 6-thiotheophylline is more active than the 6-thiotheobromine and 6-thiocaffeine. The 1,3-disubstituted compds. were more active as broncho- and coronary dilators than the 3,7-substituted compds. Maximum bronchodilator activity was achieved with relatively large alkyl groups in the 1 and 3 positions, and the 3-isobutyl derivative of 1-methyl-6-thiotheophylline was most active. Large groups in the 1-position may reduce oral absorption. Compds. with unsatd. or substituted alkyl groups in the 3-position are less bronchoactive than compds. containing the corresponding saturated or unsubstituted groups. A 1-methyl group may be essential for coronary dilator activity. All the compds. tested had low diuretic activity. 6-Thiocaffeines, in contrast to caffeine, show no stimulant properties.

IT 90230-11-8, Choline, compound with 6-thiotheophylline  
 96536-20-8, Choline, compound with 3-ethyl-1-methyl-6-thioxanthine  
 96536-21-9, Choline, compound with 1,3,8-trimethyl-6-thioxanthine  
 96652-89-0, Choline, compound with 1-ethyl-3-methyl-6-thioxanthine  
 96986-49-1, Choline, compound with 1,3-diethyl-6-thioxanthine  
 97212-71-0, Choline, compound with 8-ethyl-6-thiotheophylline  
 97212-72-1, Choline, compound with 1-methyl-3-propyl-6-thioxanthine  
 97282-72-9, Choline, compound with 3-allyl-1-methyl-6-thioxanthine  
 97406-00-3, Choline, compound with 3-isobutyl-1-methyl-6-thioxanthine  
 97406-02-5, Choline, compound with 3-butyl-1-methyl-6-thioxanthine  
 97439-87-7, Choline, compound with 1-butyl-3-methyl-6-thioxanthine  
 97616-67-6, Choline, compound with 3-butyl-1-ethyl-6-thioxanthine  
 97767-38-9, Choline, compound with 1-methyl-3-pentyl-6-thioxanthine  
 97767-40-3, Choline, compound with 1,3-dipropyl-6-thioxanthine  
 97783-97-6, Choline, compound with 3-isopentyl-1-methyl-6-thioxanthine  
 98174-21-1, Choline, compound with 3-hexyl-1-methyl-6-thioxanthine  
 98801-33-3, Choline, compound with 3-benzyl-1-methyl-6-thioxanthine  
 99688-81-0, Choline, compound with 1-methyl-3-phenethyl-6-thioxanthine  
 106802-46-4, Choline, compound with 1-methyl-3-(2-methylallyl)-6-thioxanthine

(blood vessel and bronchial dilation by)

RN 90230-11-8 CAPLUS

CN Choline, compd. with 6-thiotheophylline (6CI, 7CI) (CA INDEX NAME)

CM 1

CRN 44519-34-8

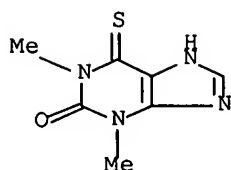
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CM 2

CRN 2398-70-1

CMF C7 H8 N4 O S



RN 96536-20-8 CAPLUS

CN Choline, compd. with 3-ethyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 44519-34-8

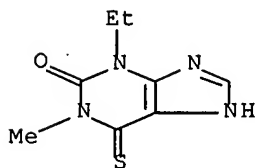
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CM 2

CRN 42458-87-7

CMF C8 H10 N4 O S



RN 96536-21-9 CAPLUS

CN Choline, compd. with 1,3,8-trimethyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 44519-34-8

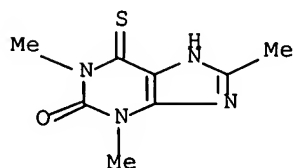
CMF C5 H13 N O

 $\text{Me}_3\text{N}-\text{CH}_2-\text{CH}_2-\text{O}^-$ 

CM 2

CRN 42459-09-6

CMF C8 H10 N4 O S



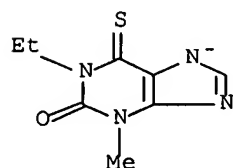
RN 96652-89-0 CAPLUS

CN Choline, compd. with 1-ethyl-3-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 96652-88-9

CMF C8 H9 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O

 $\text{Me}_3\text{N}-\text{CH}_2-\text{CH}_2-\text{OH}$ 

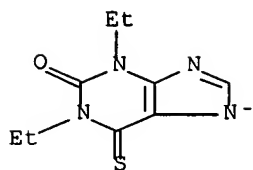
RN 96986-49-1 CAPLUS

CN Choline, compd. with 1,3-diethyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 96986-48-0

CMF C9 H11 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O

 $\text{Me}_3\text{N}-\text{CH}_2-\text{CH}_2-\text{OH}$ 

RN 97212-71-0 CAPLUS

CN Choline, compd. with 8-ethyl-6-thiotheophylline (7CI) (CA INDEX NAME)

CM 1

CRN 44519-34-8

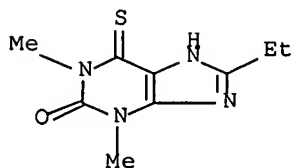
CMF C5 H13 N O

 $\text{Me}_3\text{N}-\text{CH}_2-\text{CH}_2-\text{O}^-$ 

CM 2

CRN 42459-10-9

CMF C9 H12 N4 O S



RN 97212-72-1 CAPLUS

CN Choline, compd. with 1-methyl-3-propyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 44519-34-8

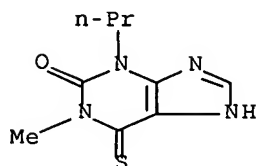
CMF C5 H13 N O

 $\text{Me}_3\text{N}-\text{CH}_2-\text{CH}_2-\text{O}^-$ 

CM 2

CRN 42458-88-8

CMF C9 H12 N4 O S



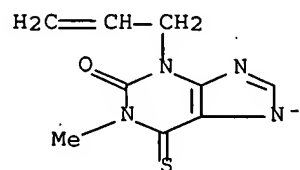
RN 97282-72-9 CAPLUS

CN Choline, compd. with 3-allyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 97282-71-8

CMF C9 H9 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O

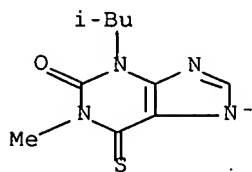
 $\text{Me}_3\text{N}-\text{CH}_2-\text{CH}_2-\text{OH}$ 

RN 97406-00-3 CAPLUS

CN Choline, compd. with 3-isobutyl-1-methyl-6-thioxanthine (6CI, 7CI) (CA INDEX NAME)

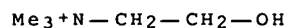
CM 1

CRN 97405-99-7  
CMF C10 H13 N4 O S



CM 2

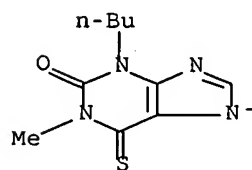
CRN 62-49-7  
CMF C5 H14 N O



RN 97406-02-5 CAPLUS  
CN Choline, compd. with 3-butyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

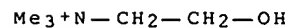
CM 1

CRN 97406-01-4  
CMF C10 H13 N4 O S



CM 2

CRN 62-49-7  
CMF C5 H14 N O

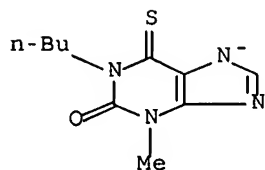


RN 97439-87-7 CAPLUS  
CN Choline, compd. with 1-butyl-3-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

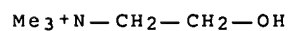


CRN 97439-86-6  
CMF C10 H13 N4 O S



CM 2

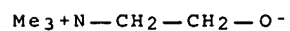
CRN 62-49-7  
CMF C5 H14 N O



RN 97616-67-6 CAPLUS  
CN Choline, compd. with 3-butyl-1-ethyl-6-thioxanthine (7CI) (CA INDEX NAME)

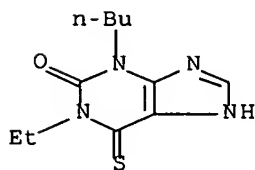
CM 1

CRN 44519-34-8  
CMF C5 H13 N O



CM 2

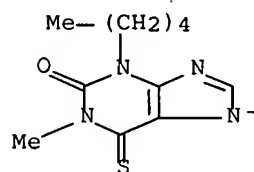
CRN 42459-03-0  
CMF C11 H16 N4 O S



RN 97767-38-9 CAPLUS  
CN Choline, compd. with 1-methyl-3-pentyl-6-thioxanthine (7CI) (CA INDEX NAME)

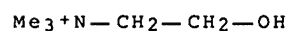
CM 1

CRN 97767-37-8  
CMF C11 H15 N4 O S



CM 2

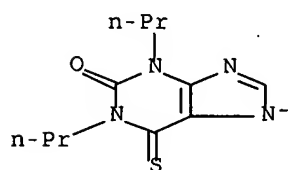
CRN 62-49-7  
CMF C5 H14 N O



RN 97767-40-3 CAPLUS  
CN Choline, compd. with 1,3-dipropyl-6-thioxanthine (7CI) (CA INDEX NAME)

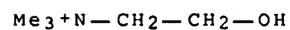
CM 1

CRN 97767-39-0  
CMF C11 H15 N4 O S



CM 2

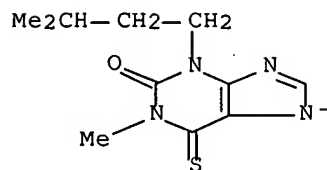
CRN 62-49-7  
CMF C5 H14 N O



RN 97783-97-6 CAPLUS  
CN Choline, compd. with 3-isopentyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

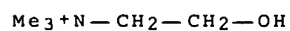
CM 1

CRN 97783-96-5  
CMF C11 H15 N4 O S



CM 2

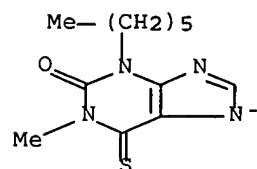
CRN 62-49-7  
CMF C5 H14 N O



RN 98174-21-1 CAPLUS  
CN Choline, compd. with 3-hexyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

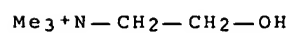
CM 1

CRN 98174-20-0  
CMF C12 H17 N4 O S



CM 2

CRN 62-49-7  
CMF C5 H14 N O

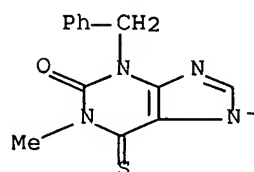


RN 98801-33-3 CAPLUS  
CN Choline, compd. with 3-benzyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 98801-32-2

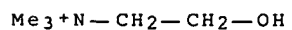
CMF C13 H11 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O



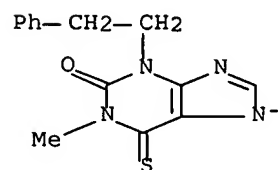
RN 99688-81-0 CAPLUS

CN Choline, compd. with 1-methyl-3-phenethyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 99688-80-9

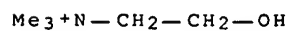
CMF C14 H13 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O



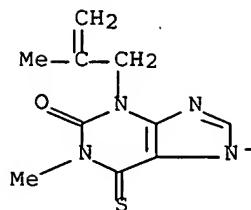
RN 106802-46-4 CAPLUS

CN Choline, compd. with 1-methyl-3-(2-methylallyl)-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN . 106802-45-3

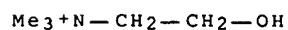
CMF C10 H11 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O



IT 96536-20-8, Xanthine, 3-ethyl-1-methyl-6-thio-, compound with choline 96986-49-1, Xanthine, 1,3-diethyl-6-thio-, compound with choline 97212-72-1, Xanthine, 1-methyl-3-propyl-6-thio-, compound with choline 97406-02-5, Xanthine, 3-butyl-1-methyl-6-thio-, compound with choline 97439-87-7, Xanthine, 1-butyl-3-methyl-6-thio-, compound with choline 97616-67-6, Xanthine, 3-butyl-1-ethyl-6-thio-, compound with choline 97767-38-9, Xanthine, 1-methyl-3-pentyl-6-thio-, compound with choline 97783-97-6, Xanthine, 3-isopentyl-1-methyl-6-thio-, compound with choline 98174-21-1, Xanthine, 3-hexyl-1-methyl-6-thio-, compound with choline 98801-33-3, Xanthine, 3-benzyl-1-methyl-6-thio-, compound with choline 99688-81-0, Xanthine, 1-methyl-3-phenethyl-6-thio-, compound with choline 106802-46-4, Xanthine, 1-methyl-3-(2-methylallyl)-6-thio-, compound with choline 856653-25-3, Theophylline, 8-ethyl-6-thio-, compound with choline 878790-85-3, Xanthine, 1,3,8-trimethyl-6-thio-, compound with choline 878790-86-4, Xanthine, 1-ethyl-3-methyl-6-thio-, compound with choline 878790-87-5, Xanthine, 1,3-dipropyl-6-thio-, compound with choline 878794-41-3, Theophylline, 6-thio-, compound with choline 879632-11-8, Xanthine, 3-allyl-1-ethyl-6-thio-, compound with choline

(blood-vessel and bronchial dilation by)

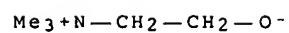
RN 96536-20-8 CAPLUS

CN Choline, compd. with 3-ethyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 44519-34-8

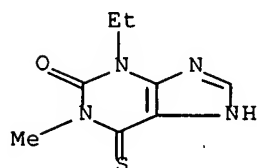
CMF C5 H13 N O



CM 2

CRN 42458-87-7

CMF C8 H10 N4 O S



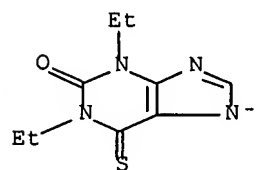
RN 96986-49-1 CAPLUS

CN Choline, compd. with 1,3-diethyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 96986-48-0

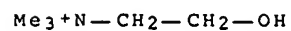
CMF C9 H11 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O



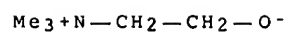
RN 97212-72-1 CAPLUS

CN Choline, compd. with 1-methyl-3-propyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 44519-34-8

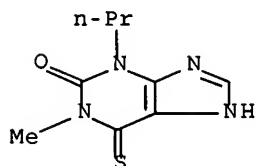
CMF C5 H13 N O



CM 2

CRN 42458-88-8

CMF C9 H12 N4 O S



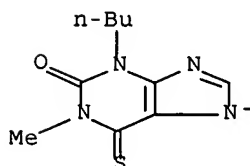
RN 97406-02-5 CAPLUS

CN Choline, compd. with 3-butyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 97406-01-4

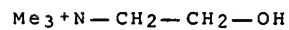
CMF C10 H13 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O



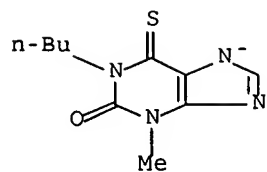
RN 97439-87-7 CAPLUS

CN Choline, compd. with 1-butyl-3-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 97439-86-6

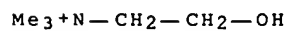
CMF C10 H13 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O



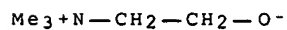
RN 97616-67-6 CAPLUS

CN Choline, compd. with 3-butyl-1-ethyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 44519-34-8

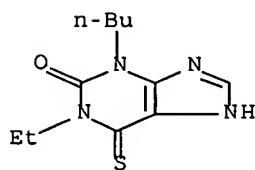
CMF C5 H13 N O



CM 2

CRN 42459-03-0

CMF C11 H16 N4 O S



RN 97767-38-9 CAPLUS

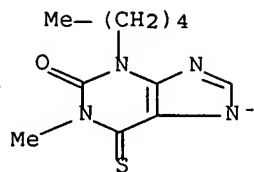
CN Choline, compd. with 1-methyl-3-pentyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 97767-37-8

CMF C11 H15 N4 O S

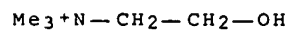




CM 2

CRN 62-49-7

CMF C5 H14 N O



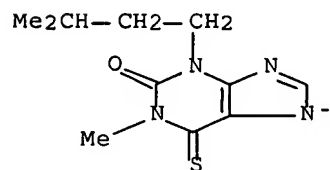
RN 97783-97-6 CAPLUS

CN Choline, compd. with 3-isopentyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 97783-96-5

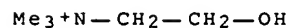
CMF C11 H15 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O



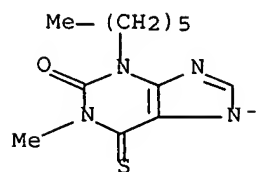
RN 98174-21-1 CAPLUS

CN Choline, compd. with 3-hexyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 98174-20-0

CMF C12 H17 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O

Me<sub>3</sub>N—CH<sub>2</sub>—CH<sub>2</sub>—OH

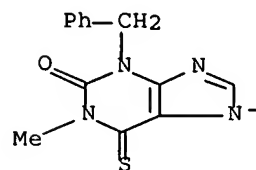
RN 98801-33-3 CAPLUS

CN Choline, compd. with 3-benzyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 98801-32-2

CMF C13 H11 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O

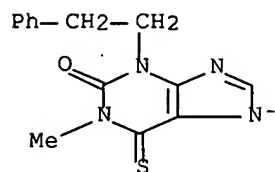
Me<sub>3</sub>N—CH<sub>2</sub>—CH<sub>2</sub>—OH

RN 99688-81-0 CAPLUS

CN Choline, compd. with 1-methyl-3-phenethyl-6-thioxanthine (7CI) (CA INDEX NAME)

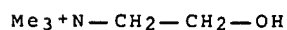
CM 1

CRN 99688-80-9  
CMF C14 H13 N4 O S



CM 2

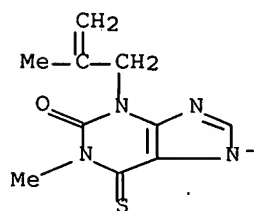
CRN 62-49-7  
CMF C5 H14 N O



RN 106802-46-4 CAPLUS  
CN Choline, compd. with 1-methyl-3-(2-methylallyl)-6-thioxanthine (7CI) (CA INDEX NAME)

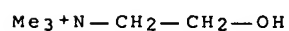
CM 1

CRN 106802-45-3  
CMF C10 H11 N4 O S



CM 2

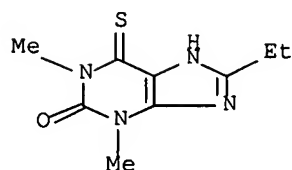
CRN 62-49-7  
CMF C5 H14 N O



RN 856653-25-3 CAPLUS  
CN Theophylline, 8-ethyl-6-thio-, compd. with choline (7CI) (CA INDEX NAME)

CM 1

CRN 42459-10-9  
CMF C9 H12 N4 O S



CM 2

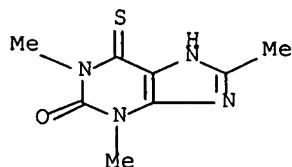
CRN 62-49-7  
CMF C5 H14 N O

$\text{Me}_3\text{N}-\text{CH}_2-\text{CH}_2-\text{OH}$

RN 878790-85-3 CAPLUS  
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1,3,6,7-tetrahydro-1,3,8-trimethyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 42459-09-6  
CMF C8 H10 N4 O S



CM 2

CRN 62-49-7  
CMF C5 H14 N O

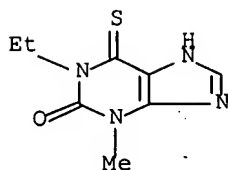
$\text{Me}_3\text{N}-\text{CH}_2-\text{CH}_2-\text{OH}$

RN 878790-86-4 CAPLUS  
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1-ethyl-1,3,6,7-tetrahydro-3-methyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 42459-00-7

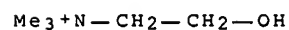
CMF C8 H10 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O



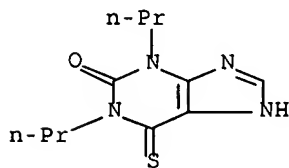
RN 878790-87-5 CAPLUS

CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1,3,6,7-tetrahydro-1,3-dipropyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 42459-06-3

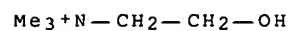
CMF C11 H16 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O



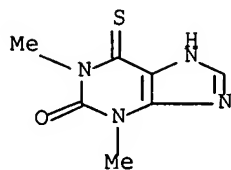
RN 878794-41-3 CAPLUS

CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 2398-70-1

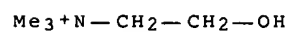
CMF C7 H8 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O



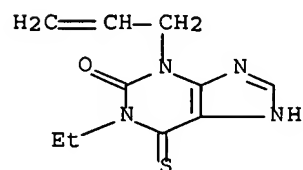
RN 879632-11-8 CAPLUS

CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1-ethyl-1,3,6,7-tetrahydro-3-(2-propenyl)-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 42459-02-9

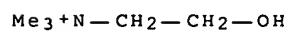
CMF C10 H12 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O



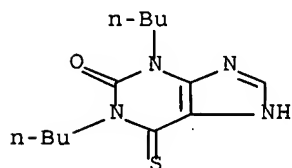
IT 40915-18-2, Xanthine, 1,3-dibutyl-6-thio- 42458-94-6,

Xanthine, 3-(3-methoxypropyl)-1-methyl-6-thio- 42458-99-1,  
 Xanthine, 3-furfuryl-1-methyl-6-thio- 42459-02-9, Xanthine,  
 3-allyl-1-ethyl-6-thio- 42459-04-1, Xanthine,  
 1-ethyl-3-isobutyl-6-thio- 93263-24-2, Xanthine,  
 3-isobutyl-6-thio-

(sodium derivative, blood-vessel and bronchial dilation by)

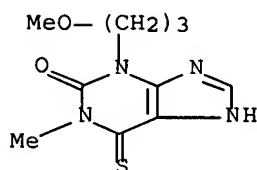
RN 40915-18-2 CAPLUS

CN 2H-Purin-2-one, 1,3-dibutyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



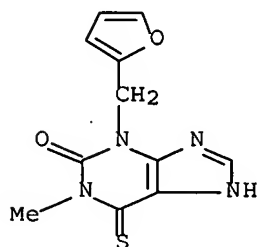
RN 42458-94-6 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(3-methoxypropyl)-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



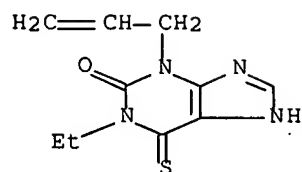
RN 42458-99-1 CAPLUS

CN 2H-Purin-2-one, 3-(2-furanylmethyl)-1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



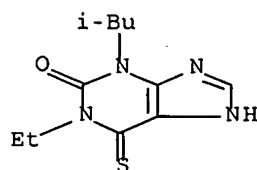
RN 42459-02-9 CAPLUS

CN 2H-Purin-2-one, 1-ethyl-1,3,6,7-tetrahydro-3-(2-propenyl)-6-thioxo- (9CI) (CA INDEX NAME)



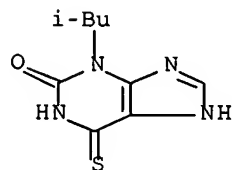
RN 42459-04-1 CAPLUS

CN 2H-Purin-2-one, 1-ethyl-1,3,6,7-tetrahydro-3-(2-methylpropyl)-6-thioxo-  
(9CI) (CA INDEX NAME)



RN 93263-24-2 CAPLUS

CN Xanthine, 3-isobutyl-6-thio- (7CI) (CA INDEX NAME)



L57 ANSWER 107 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1962:38398 CAPLUS Full-text

DOCUMENT NUMBER: 56:38398

ORIGINAL REFERENCE NO.: 56:7262f-i,7263a-c

TITLE: Preparation and peracid oxidation of  
2-(p-dimethylamino)styrylpyridine

AUTHOR(S): Pentimalli, L.

CORPORATE SOURCE: Univ. Bologna, Italy

SOURCE: Tetrahedron (1961), 14, 151-60

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

ED Entered STN: 22 Apr 2001

GI For diagram(s), see printed CA Issue.

AB cf. CA 54, 21087a. -In substituted pyridines electronic interaction between an electron-donor substituent and the pyridine nucleus is greatest when the substituent is bonded directly to the nucleus, but is decreased when the bonding takes place through a system of double bonds. It was shown that interaction effects between the NMe<sub>2</sub> group and the pyridine ring in the title compound, 2-(p-Me<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CH:CH)C<sub>5</sub>H<sub>4</sub>N (I) are small. KOH (1.0 g.), 2.2 g. 2-MeC<sub>5</sub>H<sub>4</sub>NO, and 4.3 g. p-Me<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CHO refluxed gently 6 hrs. in 6 ml. anhydrous C<sub>5</sub>H<sub>5</sub>N, the cooled mixture stirred 20 min. in 100 ml. cold H<sub>2</sub>O, the H<sub>2</sub>O-washed



and dried precipitate shaken with 30 ml. cold Me<sub>2</sub>CO and filtered yielded 57% bright yellow II, m. 200-1°, showing the bathochromic shift of conjugated substituted pyridine 1-oxides. II (4 g.) in 80 ml. AcOH at 90° stirred 20 min. with gradual addition of 6 g. Fe powder at 100°, the mixture kept 15 min. and the cooled mixture made strongly alkaline by addition of dilute NaOH, the washed and dried powdered product extracted twice with 50 ml. boiling C<sub>6</sub>H<sub>6</sub> and the residue on evaporation (m. 136-8°) recrystd. from MeOH yielded 60% I, m. 139°. In strongly acidic medium both pyridine and amine N atoms undergo protonation, impeding the conjugative interaction with consequent decrease of absorption. I (1.0 g.) in 8 ml. CHCl<sub>3</sub> at 15° slowly treated with 0.7 g. BzO<sub>2</sub>H in CHCl<sub>3</sub>, the mixture kept 16 hrs. and shaken with saturated aqueous Na<sub>2</sub>CO<sub>3</sub>, the dried solution (anhydrous Na<sub>2</sub>CO<sub>3</sub>) filtered and the solvent evaporated gave colorless plates of 2-[p-Me<sub>2</sub>N(O)C<sub>6</sub>H<sub>4</sub>CH:CH]C<sub>5</sub>H<sub>4</sub>N, m. 100° (decomposition) (C<sub>6</sub>H<sub>6</sub>). I (1.0 g.) in 10 ml. CHCl<sub>3</sub> at 15° treated slowly with 1.7 g. BzO<sub>2</sub>H in CHCl<sub>3</sub>, kept 16 hrs., and the product isolated gave 2-[p-Me<sub>2</sub>N(O)C<sub>6</sub>H<sub>4</sub>CH:CH]C<sub>5</sub>H<sub>4</sub>NO, m. 148° (C<sub>5</sub>H<sub>5</sub>N), also obtained by oxidation of 4 g. II in 40 ml. CHCl<sub>3</sub> with 2.76 g. BzO<sub>2</sub>H in CHCl<sub>3</sub>. Condensation of 4.7 g. α-MeC<sub>5</sub>H<sub>4</sub>N with 4.6 g. BzH in 2.9 ml. AcOH containing 4.8 ml. Ac<sub>2</sub>O gave 2(PhCH:CH)C<sub>5</sub>H<sub>4</sub>N, m. 89-90°. The corresponding 2(PhCH:CH)C<sub>5</sub>H<sub>4</sub>NO was obtained by condensation of 2.2 g. 2-MeC<sub>5</sub>H<sub>4</sub>NO with 3 g. BzH with KOME in 5 ml. MeOH to give material, m. 162-3° (C<sub>6</sub>H<sub>6</sub>), also prepared by oxidation of 7.2 g. base with 6.3 ml. 36% H<sub>2</sub>O<sub>2</sub> in 25.7 ml. AcOH. It was concluded that the 1st O atom in the stepwise oxidation of I is bonded only to the amino N atom and the 2nd to the pyridine ring N atom. As with the corresponding azo derivative, the electron d. remained highest at the NH<sub>2</sub> N atom in comparison with the d. at the pyridine N atom.

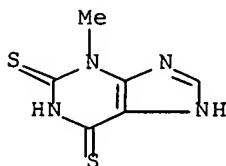
IT 33285-77-7P, Xanthine, 3-methyl-2,6-dithio-

RL: PREP (Preparation)

(preparation of)

RN 33285-77-7 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)



L57 ANSWER 108 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1962:25096 CAPLUS Full-text

DOCUMENT NUMBER: 56:25096

ORIGINAL REFERENCE NO.: 56:4762b-h

TITLE: Synthesis and properties of 3-methylpurines

AUTHOR(S): Bergmann, Felix; Levin, Gershon; Kalmus, Abraham; Kwietny, Hanna

CORPORATE SOURCE: Hebrew Univ.-Hadassah Med. School, Jerusalem, Israel

SOURCE: Journal of Organic Chemistry (1961), 26, 1504-8

CODEN: JOCEAH; ISSN: 0022-3263

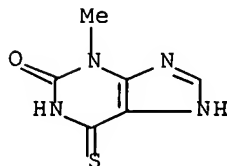
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

ED Entered STN: 22 Apr 2001

AB A series of substituted purines was prepared and, by comparison of their ultraviolet spectra, it was deduced that 3-methylhypoxanthine (I), 8-hydroxy-3-methyl-6-purinone (II), 3-methyl-8 hydroxypurine (III), 3-methylpurine-6-

RN 33285-76-6 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 109 OF 116 . CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1962:18329 CAPLUS Full-text  
 DOCUMENT NUMBER: 56:18329  
 ORIGINAL REFERENCE NO.: 56:3480c-i,3481a-b  
 TITLE: Synthesis of 8-substituted purines  
 AUTHOR(S): Bergmann, F.; Tamari, M.  
 CORPORATE SOURCE: Hebrew Univ., Jerusalem, Israel  
 SOURCE: Journal of the Chemical Society (1961) 4468-72  
 CODEN: JCSOA9; ISSN: 0368-1769  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 OTHER SOURCE(S): CASREACT 56:18329

ED Entered STN: 22 Apr 2001

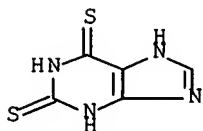
AB Condensation of an acetamidine salt with an appropriate derivative of 4,5-diaminopyrimidine in the absence of a solvent led directly to high yields of the 8-substituted purines (I). General procedure. A mixture of a 4,5diaminopyrimidine and 2 equivs. MeC(:NH)NH<sub>2</sub>.HCl (II.HCl) heated to 180-90° (homogeneous melt was formed and NH<sub>3</sub> was evolved), when reaction ceased, the melt dissolved in N NaOH, the solution decolorized with C, and acidified with AcOH to pH 6 gave the I, all decomposing above 310° [substituents at 2-, 6-, and 8-position, reaction time in min., % yield, λ (mμ) at pH 8.0, R<sub>f</sub> in 85:10:5 95% EtOH-H<sub>2</sub>OAcOH (solvent A), 70:20:10 95% EtOH-pyridine-H<sub>2</sub>O (solvent B), and 65:25:10 iso-PrOH-HCONMe<sub>2</sub>-10% aqueous NH<sub>3</sub> (solvent C) given]: H, OH, Me, 60, 56 (the yield was improved by addition of 2 equivs. anhydrous NaOAc), 2.52, 0.57, 0.70, --; H, OH, Me, 60, 67 (with II.AcOH), --, --, --, --; OH, OH, Me, 30, 94, 240 and 275, 0.54, 0.60, 0.42; OH, SH, Me (III), 35, 83 (the yield was improved by addition of 2 equivs. anhydrous NaOAc) (the same compound was also prepared in 90% yield from 8-methylxanthine with P2S<sub>5</sub>), 251 and 344, 0.50, 0.56, 0.57; SH, OH, Me, 30, 77, 235 and 280, 0.45, 0.74, 0.61; SH, SH, Me, 25, 65 (the yield was improved with 2 equivs. anhydrous NaOAc), 247 and 285, and 351, 0.53, 0.59, 0.71; SH, SH, Me (IV), 25, 86 (with II.AcOH), --, --, --, --; SH, NH<sub>2</sub>, Me (V), 30, 66 (isolated as the sulfate), 230 and 251, and 280, 0.61, 0.67, --; H, OH, Ph, 70, 50, 291, 0.58, 0.79, --; H, OH, Ph, 70, 78 (with II.AcOH), --, --, --; OH, OH, Ph, 40, 80, 228 and 309, 0.52, 0.66, --. Also were prepared 92% 3,8-dimethylxanthine (VI), λ (pH 8.0) 275 m, R<sub>f</sub> 0.64 (in A), 0.79 (in B), and 0.68 (in C), and 88% 3,8-dimethyl-2-mercaptioxanthine (VII), λ (pH 8.0), 233 and 288 mμ, R<sub>f</sub> 0.60 (in A) and 0.84 (in B). N:C(OH).-N:C(NH<sub>2</sub>).C(NH<sub>2</sub>):CH (VIII) (Kalmus and Bergmann, CA 55, 12418h) (1 g.), 1 g. II.HCl, and 0.8 g. anhydrous NaOAc heated 20 min. at 140-5, the resulting cake dissolved in 10% aqueous NH<sub>3</sub>, the solution boiled with C, filtered, and the filtrate kept 24 hrs. in a cold room gave 0.65 g.

inseparable mixture of VIII and 2-hydroxy-8-methylpurine (IX), (pH 8.0) 307 m. III (5 g.) and 1.5 g. (wet weight) Raney Ni in 25 ml. 5% aqueous NH<sub>3</sub> refluxed 80 min., filtered, the filtrate adjusted to pH 2 with HNO<sub>3</sub>, and kept 2 months at room temperature gave IX.HNO<sub>3</sub>. If the above ammoniacal solution was acidified with H<sub>2</sub>SO<sub>4</sub>, IX decomposed quant. The same result was obtained when an ammoniacal solution of IX was evaporated to dryness, the residue extracted with absolute EtOH, and the mixture acidified with 1% alc.-H<sub>2</sub>SO<sub>4</sub>. V (580 mg.) and 1.5 g. (wet weight) Raney Ni in 100 ml. 5% aqueous NH<sub>2</sub> refluxed 2 hrs., filtered hot, and the filtrate cooled gave 300 mg. 8-methyladenine, Rf 0.57 (in A), 0.67 (in B), and 0.64 (in C). 8-Methylhypoxanthine (1.3 g.), 5 g. P<sub>2</sub>S<sub>5</sub>, and 50 ml. dry pyridine refluxed 4 hrs., concentrated in vacuo, the residue extracted with 37 NaOH, filtered, the solution concentrated in vacuo, and kept overnight at 0° gave 1.1 g. 6-mercapto-8-methylpurine, decomposed above 310° (H<sub>2</sub>O), (pH 8.0) 232 and 316 m, Rf 0.64 (in A) and 0.71 (in C). VII (1 g.) and 0.7 ml. MeI stirred 30 min. at room temperature in 10 ml. 0.5N NaOH gave 0.95 g. 3,8-dimethyl-2-(methylthio)hypoxanthine, decomposed at 312-15° (H<sub>2</sub>O), Rf 0.73 (in B). VII (2 g.) and 6 g. (wet weight) Raney Ni in 50 ml. 5% aqueous NH<sub>3</sub> refluxed 2 hrs., filtered, and concentrated in vacuo gave 1.4 g. 3,8-dimethylhypoxanthine, decomposed at 300° (EtOH), Rf 0.6 (in B). NH.CO.NMe.C(NH<sub>2</sub>):C-(NH<sub>2</sub>).CS (X) and II.HCl or II.ACOH heated at 150-200° gave only X and tars. VI treated with P<sub>2</sub>S<sub>5</sub> in pyridine, concentrated in vacuo, the residue decomposed with cold dilute aqueous NH<sub>3</sub>, the mixture filtered, and the filtrate adjusted to pH 6 with AcOH gave only X, λ (pH 8.0) 249 and 344 mμ, Rf 0.33 (in A). IV (1 g.) and 2.5 g. Raney Ni in 50 ml. 5% aqueous NH<sub>3</sub> refluxed 70 min., filtered, the filtrate concentrated in vacuo, and kept overnight gave 150 mg. 8-methylpurine, λ (pH 8.0) 266 mμ, Rf 0.75 (in A).

IT 5437-25-2P, Xanthine, dithio- 91184-09-7P, Xanthine,  
8-methyl-2-thio- 91184-10-0P, Xanthine, 8-methyl-6-thio-  
91725-06-3P, Xanthine, 3,8-dimethyl-2-thio-  
RL: PREP (Preparation)  
(preparation of)

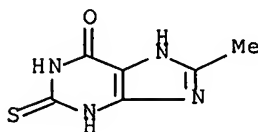
RN 5437-25-2 CAPLUS

CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



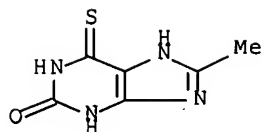
RN 91184-09-7 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-8-methyl-2-thioxo- (9CI) (CA INDEX NAME)

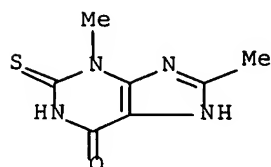


RN 91184-10-0 CAPLUS

CN Xanthine, 8-methyl-6-thio- (7CI) (CA INDEX NAME)



RN 91725-06-3 CAPLUS  
 CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3,8-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 110 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1961:60865 CAPLUS Full-text  
 DOCUMENT NUMBER: 55:60865  
 ORIGINAL REFERENCE NO.: 55:11652a-d  
 TITLE: Thioxanthines with potent bronchodilator and coronary dilator properties  
 AUTHOR(S): Armitage, A. K.; Boswood, Janet; Large, B. J.  
 CORPORATE SOURCE: May and Baker, Dagenham, UK  
 SOURCE: British Journal of Pharmacology and Chemotherapy (1961), 16, 59-76  
 CODEN: BJPCAL; ISSN: 0366-0826  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 ED Entered STN: 22 Apr 2001  
 AB The pharmacol. properties of 2 new compds., choline 6-thiotheophyllinate (I) and the choline salt of 3-isobutyl-1-methyl-6-thioxanthine (M & B, 5924) (II) are described. As bronchodilators on the isolated guinea pig tracheal ring preparation, I and II were 57 and 5 times, resp., more active than choline theophyllinate (III). In protective effect against bronchioconstrictor aerosols, III (50 and 100 mg./kg., i.p.) was almost identical with that of I. II (100 mg./kg. orally) appeared to give more protection than III (200 mg./kg.). I and II had very little antihistaminic and antiacetylcholine activity. In cardiovascular studies on the anesthetized cats and dogs, all 3 compds. caused a transient fall in blood pressure. I and II were more potent than III as coronary dilators on the dog heart-lung preparation. As diuretics they were less potent. In doses up to 20 mg./kg., III increased the voluntary locomotor activity of mice. A 50% increase was produced by 12 mg. of I and II each/kg. However, other doses from 5 to 80 mg./kg. either decreased motor activity or had no effect. A 50% decrease in motor activity was produced by 32 mg. I/kg. and by 30 mg. II/kg. Toxic doses of III caused intense excitement and convulsions, whereas toxic doses of the thioxanthines caused sedation. Death in all cases was due to respiratory failure. In dogs, I in doses as high as 120 mg./kg., orally, caused no ill effects; II at 60 and 80 mg./kg. caused vomiting and retching lasting for about 1 h. II given i.v. to

dogs in doses up to 3 mg./kg. caused vomiting, retching, excitation, and restlessness in contrast to the sedation seen in mice.

IT 857018-10-1, Xanthine, 3-isobutyl-1-methyl-6-thio-, compound with choline 878794-41-3, Theophylline, 6-thio-, compound with choline (pharmacol. of)

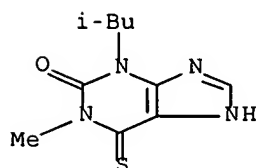
RN 857018-10-1 CAPLUS

CN Xanthine, 3-isobutyl-1-methyl-6-thio-, compd. with choline (6CI) (CA INDEX NAME)

CM 1

CRN 42458-91-3

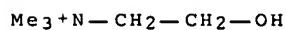
CMF C10 H14 N4 O S



CM 2

CRN 62-49-7

CMF C5 H14 N O



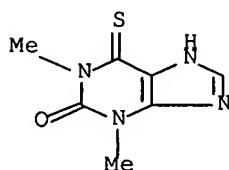
RN 878794-41-3 CAPLUS

CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 2398-70-1

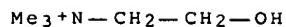
CMF C7 H8 N4 O S



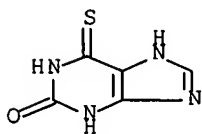
CM 2

CRN 62-49-7

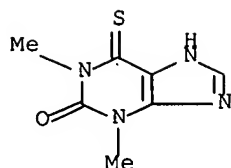
CMF C5 H14 N O



L57 ANSWER 111 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1961:56289 CAPLUS Full-text  
 DOCUMENT NUMBER: 55:56289  
 ORIGINAL REFERENCE NO.: 55:10804b-d  
 TITLE: 1,3-Dialkyl-6-thioxanthines: a new series of  
 bronchodilators and coronary vasodilators  
 AUTHOR(S): Armitage, A. K.; Wooldridge, K. R. H.  
 CORPORATE SOURCE: May & Baker, Ltd., Dagenham, UK  
 SOURCE: Nature (London, United Kingdom) (1960), 188,  
 1107-8  
 CODEN: NATUAS; ISSN: 0028-0836  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 ED Entered STN: 22 Apr 2001  
 AB Thioxanthines were prepared from the corresponding xanthines by refluxing for  
 several hrs. with P2S5 in pyridine. Thionation occurred in the 6-position  
 only. The choline salt of 3-isobutyl-1-methyl-6-thioxanthine (I), the most  
 active derivative in vitro for relaxation of the bronchial muscle and dilation  
 of the coronary vessels, is pale-yellow, crystalline, solid, m. 145-7°, and  
 >50% soluble in H2O at 20°. Choline 6-thiotheophyllinate (II), m. 146-9°, has  
 similar solubility The thio derivs. are more active in vitro than in vivo. I  
 is more active than II in dilating the coronary vessels of the dog heart-lung  
 preparation or of the anesthetized dog, and in dilating the vessels of the  
 hind leg of the dog perfused with heparinized blood.  
 IT 2002-59-7, Xanthine, 6-thio-  
 (1,3-dialkyl derivs., as bronchodilators and coronary vasodilators)  
 RN 2002-59-7 CAPLUS  
 CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



IT 878794-41-3, Theophylline, 6-thio-, compound with choline  
 (as bronchodilator and coronary vasodilator)  
 RN 878794-41-3 CAPLUS  
 CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1,3,6,7-tetrahydro-  
 1,3-dimethyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 2398-70-1  
 CMF C7 H8 N4 O S



CM 2

CRN 62-49-7  
CMF C5 H14 N O

Me<sub>3</sub>N—CH<sub>2</sub>—CH<sub>2</sub>—OH

L57 ANSWER 112 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1959:39968 CAPLUS Full-text

DOCUMENT NUMBER: 53:39968

ORIGINAL REFERENCE NO.: 53:7191g-i, 7192a-i

TITLE: Potential purine antagonists. XIII. Synthesis of some 8-methylpurines

AUTHOR(S): Koppel, Henry C.; Robins, Rolland K.

CORPORATE SOURCE: Arizona State Coll., Tempe

SOURCE: Journal of Organic Chemistry (1958), 23, 1457-60

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 53:39968

ED Entered STN: 22 Apr 2001

AB cf. C.A. 53, 1366a. Use of Ac<sub>2</sub>O as a general cyclizing agent for 4,5-diaminopyrimidines was investigated. A number of new 8-methylpurines were prepared 4,5-Diamino-6-hydroxypyrimidine (I) with Ac<sub>2</sub>O gave 70% 6-hydroxy-8-methylpurine (II). I (15 g.) refluxed 80 min. in 250 ml. Ac<sub>2</sub>O, excess Ac<sub>2</sub>O removed in vacuo, the sirupy residue refluxed 10 min. in 250 ml. 1.5N NaOH, treated with C, cooled, acidified, and separated gave 14 g. II.H<sub>2</sub>O, m. above 300°. II (35 g.) added to 500 ml. POCl<sub>3</sub> and 50 ml. PhNMe<sub>2</sub>, the mixture refluxed 5.5 hrs., excess POCl<sub>3</sub> removed, the residue poured on ice, made strongly basic, left 20 min., extracted with Et<sub>2</sub>O, the solution acidified, continuously extracted with Et<sub>2</sub>O, and concentrated gave 18 g. 6-chloro-8-methylpurine (III), m. 212-13° (PhMe). III (5 g.) refluxed 1 hr. with 150 ml. alc. containing 10 g. CS(NH<sub>2</sub>)<sub>2</sub>, chilled, filtered, the product refluxed with 150 ml. dilute NaOH, and acidified gave 3.9 g. 8-methyl-6-purinethiol (IV), m. above 300° (H<sub>2</sub>O). IV (5 g.) refluxed 6 hrs. with 100 ml. H<sub>2</sub>O containing 15 g. Raney Ni, the Ni removed, washed with 50 ml. boiling H<sub>2</sub>O, the combined filtrate and washings evaporated to dryness, and crystallized gave 3.2 g. 8-methylpurine (C<sub>6</sub>H<sub>6</sub>-heptane-MeOH). III (5 g.) heated 2 hrs. with 50 ml. H<sub>2</sub>O containing 50 ml. 40% MeNH<sub>2</sub> gave 3.8 g. 6-methylamino-8-methylpurine, m. above 300° (H<sub>2</sub>O). III (5 g.) heated 2 hrs. with 150 ml. alc. and 9 g. p-ClC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>NH<sub>2</sub> gave 4.2 g. 8-methyl-6-(p-chlorobenzylamino)purine, m. above 300° (alc.). III (5 g.) heated 3 hrs. with 150 ml. alc. and 10 g. 2,4-Cl<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>NH<sub>2</sub> gave 4 g. 6-(2,4-dichlorobenzylamino)-8-methylpurine, m. 286-7° (alc.). IV (5 g.) in 100 ml. hot H<sub>2</sub>O containing 5 g. KOH treated 3 hrs. with 4

g. MeI, the pH adjusted to 7, and cooled gave 3 g. 6-methylthio-8-methylpurine, m. 223-4° (C<sub>6</sub>H<sub>6</sub>-heptane-MeOH). The following 6-alkylthio-8-methylpurines were prepared by a general method as shown below. IV (5 g.) heated 0.5 hr. with 75 ml. H<sub>2</sub>O, 3 g. KOH, and 10 g. EtSH, the pH adjusted to 7 with dilute HCl, and the crude product collected gave 3.6 g. 6-ethylthio-8-methylpurine (V), m. 206-7° (EtOAc-heptane). The following 6-alkylthio analogs of V were similarly prepared (alkyl given): Pr, m. 214-15° (C<sub>6</sub>H<sub>6</sub>-heptane); iso-Pr, m. 256-7° (EtOAc-heptane); Bu, m. 179-80° (C<sub>6</sub>H<sub>6</sub>-heptane-MeOH). 4,5-Diamino-6-hydroxy-2-mercaptopyrimidine (10 g.) refluxed 9 hrs. in 250 ml. Ac<sub>2</sub>O, cooled, the solid collected, washed, refluxed 10 min. with 250 ml. 1.5N NaOH, and acidified gave 11.5 g. 6-hydroxy-8-methyl-2-purinethiol (VI), m. above 300° (dilute AcOH). VI (20 g.) in 500 ml. 0.5N NaOH stirred with 15 g. MeI until only one phase resulted, the solution heated to 80° treated with C, acidified, and cooled gave 14 g. 6-hydroxy-8-methyl-2-methylthiopurine (VII), m. above 300° (H<sub>2</sub>O). 4,5-Diamino-6-hydroxy-2-(methylthio)pyrimidine (23 g.) refluxed 2 hrs. in 250 ml. Ac<sub>2</sub>O, excess Ac<sub>2</sub>O distilled, the residue refluxed in 250 ml. 1.5N NaOH, the solution acidified, and cooled gave 22 g. VII, identical with the above prepared specimen. VI (15 g.) refluxed 5 hrs. in 500 ml. C<sub>5</sub>H<sub>5</sub>N containing 60 g. P<sub>2</sub>S<sub>5</sub>, the excess C<sub>5</sub>H<sub>5</sub>N removed, 300 ml. H<sub>2</sub>O added, the mixture heated 3 hrs., cooled, the product collected, and repptd. twice from dilute Na<sub>2</sub>CO<sub>3</sub> with acid gave 8-methyl-2,6-purinedithiol, m. above 300°. VII (35 g.) refluxed 3.5 hrs. with 500 ml. POCl<sub>3</sub> and 70 ml. PhNEt<sub>2</sub>, excess POCl<sub>3</sub> removed in vacuo, the residue poured on ice, made basic, extracted with Et<sub>2</sub>O, the aqueous solution kept at 10°, acidified to pH 1, left 3 hrs., and the solid collected gave 21 g. 6-chloro-8-methyl-2-(methylthio)purine (VIII), m. 268-70° (PhMe). VIII (5 g.) refluxed 1 hr., cooled, the crude product dissolved in dilute KOH, and repptd. with AcOH gave 4.1 g. 8-methyl-2-methylthio-6-purinethiol (IX), m. above 300° (dilute AcOH). IX (5 g.) in 150 ml. alc. heated with 10 g. p-ClC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>NH<sub>2</sub> until the volume reached 75 ml. and cooled gave 5.4 g. 6-(p-chlorobenzylamino)-8-methyl-2-(methylthio)purine, m. 265-6° (alc.). VIII (5 g.) in 100 ml. alc. heated with 10 g. Me<sub>2</sub>NNH<sub>2</sub> until the volume was reduced to half and cooled gave 3.9 g. 6-(unsym-dimethylhydrazino)-8-methyl-2-(methylthio)purine, needles, m. 289-91° (alc.). VIII (5 g.), 125 ml. alc., and 10 g. NH<sub>4</sub>Et<sub>2</sub> similarly heated and evaporated gave 2.8 g. 6-diethylamino-8-methyl-2-(methylthio)purine, m. 216-18° (heptane-alc.). VIII (5 g.), 100 ml. 40% MeNH<sub>2</sub>, and 50 ml. H<sub>2</sub>O similarly treated gave 4 g. 8-methyl-6-methylamino-2-(methylthio)purine, m. 209° (alc.). 6-Dimethylamino-8-methyl-2-(methylthio)purine was similarly prepared 4,5,6-Triaminopyrimidine (15 g.) refluxed 2 hrs. with 150 ml. Ac<sub>2</sub>O, excess Ac<sub>2</sub>O removed, the residue dissolved in 300 ml. refluxing dilute NH<sub>4</sub>OH, the cooled solution filtered, the solid purified, and repptd. gave 12 g. 6-amino-8-methylpurine, m. above 300° (HCONMe<sub>2</sub>). 2,4,5-Triamino-6-hydroxypyrimidine (22 g.) refluxed 5 hrs. with 500 ml. 1:1 Ac<sub>2</sub>O-HC(OEt)<sub>3</sub>, distilled, the sirupy residue refluxed 10 min. in 250 ml. 2N NaOH, and acidified gave 12 g. 2-amino-6-hydroxy-8-methylpurine, m. above 300°. 2,6-Dihydroxy-4,5-diaminopyrimidine (10 g.) refluxed 12 hrs. in 250 ml. Ac<sub>2</sub>O and the crude product refluxed in 250 ml. 2N NaOH gave 10 g. 2,6-dihydroxy-8-methylpurine, m. above 300°. 4,5-Diamino-6-pyrimidinethiol (2.5 g.) refluxed 3 hrs. with 50 ml. Ac<sub>2</sub>O and the sirupy residue refluxed 10 min. in 100 ml. dilute NH<sub>4</sub>OH gave 2 g. 7-amino-2-methylthiazolo[5,4-d]pyrimidine. A general H<sub>2</sub>O-solubilizing effect of the 8-Me group as compared to the corresponding simple purine derivative was noted. This group may interfere with the intermol. H bonding forces in the crystal lattice. This effect is not noted in the parent compound, 8-methylpurine.

The ultraviolet absorption of some β-methylpurines are recorded.

IT 91184-09-7P, Xanthine, 8-methyl-2-thio- 91184-18-8P,

Xanthine, 8-methyldithio-

RL: PREP (Preparation)

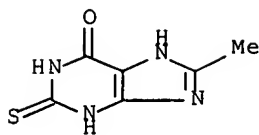
(preparation of)

RN 91184-09-7 CAPLUS

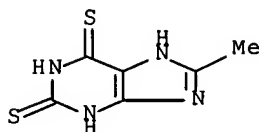
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-8-methyl-2-thioxo- (9CI) (CA INDEX



NAME)



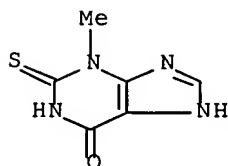
RN 91184-18-8 CAPLUS  
 CN Xanthine, 8-methyl-2,6-dithio- (7CI) (CA INDEX NAME)



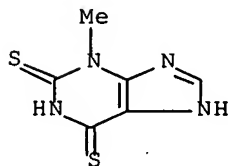
L57 ANSWER 113 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1959:34829 CAPLUS Full-text  
 DOCUMENT NUMBER: 53:34829  
 ORIGINAL REFERENCE NO.: 53:6243f-i,6244a-c  
 TITLE: Some new N-methylpurines  
 AUTHOR(S): Elion, Gertrude B.  
 CORPORATE SOURCE: Wellcome Research Labs., Tuckahoe, NY  
 SOURCE: Ciba Foundation Symposium, Chem. and Biol. Purines (1957) 39-49  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 ED Entered STN: 22 Apr 2001  
 AB Ring closure in 5-formamido-4-amino-3-methyl-2-mercapto-6-oxopyrimidine (I) gave 2-mercapto-3-methylhypoxanthine (II), which on treatment with Raney Ni provided 3-methylhypoxanthine (III). I with Raney Ni gave 5-formamido-4-amino-3-methyl-6-oxopyrimidine which underwent ring closure with formamide to form III. III with P2S5 in pyridine provided 3-methyl-6-mercaptapurine which when treated with NH4OH at 140° for 16 h. gave 3-methyladenine (IV). Excellent yields of IV were obtained by treatment of II with P2S5 to form 3-methyl-2,6-dithiopurine, which was then converted to the 6-amino derivative and treated with Raney Ni to give IV. Methylation of 5-formamido-4-amino-2-mercapto-6-oxopyrimidine (V) with Me2SO4 in aqueous alkali gave the 2-methylthio-1-Me derivative (VI), as well as a water-soluble compound believed to be 4-amino-5-formamido-2-methylthio-6-methoxypyrimidine. VI with Raney Ni gave 5-formamido-4-amino-1-methyl-6-oxopyrimidine, which was converted to 1-methylhypoxanthine (VII) by heating with HCO2H. Treatment of VII with P2S5 in Tetralin or pyridine gave 1-methyl-6-mercaptapurine (VIII). Cyclization of VI with HCO2H gave 2-methylthio-1-methylhypoxanthine, which yielded 1-methylxanthine on acid hydrolysis and 1-methylguanine on heating with NH4OH. Heating of VIII with aqueous NH3 at 140° gave 4-amino-5-imidazolecarboxamide. With alc. NH3 at 160°, VIII was converted to 6-(methylamino)purine. VI with P2S5 in pyridine gave 2-methylthio-1-methyl-6-thiopurine, which when heated with NH4OH at 140° formed 1-methyl-2,6-diaminopurine. When 6-chloropurine was methylated and then treated with NaSH, 7-methyl- and 9-methyl-6-mercaptapurines were formed. These were easily separated because of a

difference in solubility in water. 9-Methyladenine, prepared from 6-amino-2-methylthio-9-methylpurine, gave 9-methylhypoxanthine on treatment with HNO<sub>2</sub>. The UV absorption maximum (in mμ) at pH 1, 3, 7, and 11 were, for substituted hypoxanthines were (substituent given): H, 248, -, 249, 258; 1-Me, 249, -, 251, 260; 3-Me, 253, 262, 264, 265; 7-Me, 250, 255, 256, 262; 9-Me, 250, -, 250, 254. For substituted purines: 6-MeO, 254, -, 252, 261; 6-HS, 325, 323, 322, 233 (312); 1,6-Me(HS), 229(321), 233(321), 235(320), 237(321); 3,6-Me(HS), 244(334), 245(340), 245(337), 245(332); 7,6-Me(HS), 328, 328, 327, 234(315); 9,6-Me(HS), 323, 321, 320, 234(309); 6-MeS, 294, 290, 290, 290. At pH 1 and 11 for substituted adenines: H, 263, 267; 3-Me, 274, 273; 7-Me, 272, 271; 9-Me, 261, 262. 6-Methylaminopurine: 267, 272, at pH 1 and 11.

IT 28139-02-8P, Xanthine, 3-methyl-2-thio- 33285-77-7P,  
Xanthine, 3-methyldithio-  
RL: PREP (Preparation)  
(preparation of)  
RN 28139-02-8 CAPLUS  
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 33285-77-7 CAPLUS  
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)

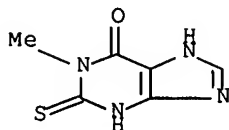


L57 ANSWER 114 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1954:11249 CAPLUS  
DOCUMENT NUMBER: 48:11249  
ORIGINAL REFERENCE NO.: 48:2093a-e  
TITLE: Substituted imidazoles and xanthenes  
INVENTOR(S): Heilbron, Ian M.; Cook, Arthur H.  
PATENT ASSIGNEE(S): Beecham Research Laboratories Ltd.  
DOCUMENT TYPE: Patent  
LANGUAGE: Unavailable  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

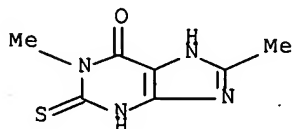
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 683523		19521203	GB 1948-21834	19480818 <--

ED Entered STN: 22 Apr 2001

- AB NH<sub>2</sub>CH(CN)CO<sub>2</sub>Et and HC(:NH)NH<sub>2</sub>.HCl refluxed 2 h. in 10:1 CHCl<sub>3</sub>-EtOH give 40% Et 4-amino-5-imidazolecarboxylate (I), m. 180-1°. I and MeNCS refluxed 1 h. in C<sub>5</sub>H<sub>5</sub>N and the solution poured into H<sub>2</sub>O gives the 4-(3-methyl-2-thioureido) analog (II) of I, m. 163°. II dissolved in 2N NaOH solution and the solution acidified with AcOH gives 1-methyl-2-thioxanthine, also prepared in 62% yield by this reaction series without isolating the intermediates. Similarly are prepared these xanthines: 1,8-di-Me, 8-Ph, 1-methyl-8-Ph (m. above 360°), 7-methyl-8-Ph [m. 340° (decomposition)], 8-benzyl-1-Ph [m. 318° (decomposition)], 1-methyl-8-(p-nitrobenzyl), 1,8-dimethyl-2-thio, 8-phenyl-2-thio (decompose above 360°), 1-methyl-8-phenyl-2-thio, 8-benzyl-1-phenyl-2-thio (m. above 360°), 8-benzyl-1,7-dimethyl-2-thio, m. above 360°, and 1,7-dimethyl-8-phenyl-2-thio, m. above 360°. This patent also includes all the intermediates of the following 2 patents. Brit. 683,593 and 683,594 cover the intermediates of types II and I, resp., of the preceding patent. The following substituted Et 5-imidazolecarboxylates were also prepared (substituents and m.ps. given): 4-amino-2-Me, 167° (decomposition) [HCl salt, m. 213-14° (decomposition)]; 4-amino-2-Ph HCl salt, 216°; 4-amino-2-benzyl HCl salt, 196° (decomposition); 4-amino-2-(p-nitrobenzyl) HCl salt, 226°, 4-amino-2-benzyl-1-Me, 145°; 4-amino-1-methyl-2-Ph, 140-2°; 2-phenyl-4-ureido, 193-5°; 2-phenyl-4-thioureido, 255°; 4-(3-acetyl-2-thioureido)-2-Ph, 225°; 1-methyl-2-phenyl-4-ureido, 193-4°; 2-methyl-4-(3-methyl-2-thioureido), 194°; 4-(3-methylureido)-2-Ph, 181-2°; 4-(3-methyl-2-thioureido)-2-Ph, 245°; 2-benzyl-4-(3-phenylureido), 187°; 2-benzyl-4-(3-phenyl-2-thioureido), 195°; 2-benzyl-1-methyl-4-(3-methyl-2-thioureido), 191°; 1-methyl-4-(3-methyl-2-thioureido)-2-Ph, 185-9°; and 4-(3-methylureido)-2-(p-nitrobenzyl), 242° (decomposition). Cf. Cook, C.A. 45, 1034bf.
- IT 91184-08-6P, Xanthine, 1-methyl-2-thio- 874519-01-4P,  
Xanthine, 1,8-dimethyl-2-thio-  
RL: PREP (Preparation)  
(preparation of)
- RN 91184-08-6 CAPLUS
- CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1-methyl-2-thioxo- (9CI) (CA INDEX NAME)

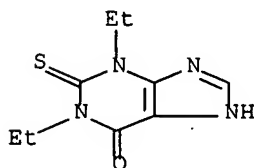


- RN 874519-01-4 CAPLUS
- CN Xanthine, 1,8-dimethyl-2-thio- (5CI) (CA INDEX NAME)



L57 ANSWER 115 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1951:61193 CAPLUS Full-text  
DOCUMENT NUMBER: 45:61193

ORIGINAL REFERENCE NO.: 45:10401e-g  
 TITLE: Diuretic activity of compounds related to xanthines, uracils, and triazines as determined in dogs  
 AUTHOR(S): Kattus, Albert A.; Newman, Elliot V.; Franklin, John  
 CORPORATE SOURCE: Johns Hopkins Univ., Baltimore, MD  
 SOURCE: Bulletin of the Johns Hopkins Hospital (1951), 89, 1-8  
 CODEN: JHHBAI; ISSN: 0097-1383  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 ED Entered STN: 22 Apr 2001  
 AB A series of 19 substituted xanthines, 1 thioxanthine, 14 uracils, 1 thiouracil, 3 triazines, 2 phenothiazines, and a substituted N-benzylaniline were tested for diuretic activity in female dogs. Urine vols. and Na excretions from dogs receiving two 0.25-0.5-g. doses in 1 day were compared with those from the same dogs prior to dosing. With Na excretion as a criterion, 1,3-diethylxanthine (I), its 2-thio analog, and its 8-bromo derivative (II) were highly diuretic, but caused emesis. Emesis was also noted with other 1,3-dialkylxanthines. In human subjects I caused diuresis and vomiting, but II had neither action. Except for 1-propyl-3-ethyl-6-aminouracil, uracil derivs. were less active than the xanthine derivs. and produced less gastrointestinal disturbance; 2,4-bis(acetamido)-s-triazine produced diuresis in a human volunteer.  
 IT 841313-23-3, Xanthine, 1,3-diethyl-2-thio- (diuretic activity of)  
 RN 841313-23-3 CAPLUS  
 CN Xanthine, 1,3-diethyl-2-thio- (5CI) (CA INDEX NAME)



L57 ANSWER 116 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1950:10067 CAPLUS Full-text  
 DOCUMENT NUMBER: 44:10067  
 ORIGINAL REFERENCE NO.: 44:1962a-i,1963a  
 TITLE: The azole series. XIV. A new synthesis of purines  
 AUTHOR(S): Cook, A. H.; Davis, A. C.; Heilbron, Ian; Thomas, G. H.  
 CORPORATE SOURCE: Imperial Coll. of Sci. and Technol., London  
 SOURCE: Journal of the Chemical Society (1949) 1071-4  
 CODEN: JCSOA9; ISSN: 0368-1769  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 OTHER SOURCE(S): CASREACT 44:10067  
 ED Entered STN: 22 Apr 2001  
 AB 4-Amino-5-carbethoxyglyoxalines and MeNCO or MeNCS gave the 4-(N-methylthioureido or ureido) compds., readily cyclized to 1-methylthioxanthines or xanthines. H<sub>2</sub>NCH<sub>2</sub>CO<sub>2</sub>Et (I) (15 g.), 30 g. PhCH<sub>2</sub>C(:NH)SCH<sub>2</sub>Ph.HCl (II), and 200 cc. dry CHCl<sub>3</sub> were refluxed 1 h., concentrated to 90 cc., 100 cc. C<sub>6</sub>H<sub>6</sub> added, and after 3 days at 0° the 20 g. HCl salt of 5-carbethoxy-2-benzyl-G (G

= 4-aminoglyoxaline) filtered, and 15 g. free base precipitated from hot H<sub>2</sub>O with NaOH; picrate, m. 221° (decomposition) (from EtOH). I (17 g.) and 15 g. PhC(:NH)OEt in 50 cc. Et<sub>2</sub>O 24 h. at room temperature gave 1.75 g. 5-carbethoxy-2-phenyl-G, m. 218° (decomposition) (from EtOH), and 0.4 g. more on concentration of the filtrate. The HCl salt, m. 216° (decomposition) (from MeOH), was obtained in 2.3-g. yield by 30 mins.' refluxing of 1.5 g. I, 3 g. PhC(:NH)SCH<sub>2</sub>Ph.HCl, and 25 cc. CHCl<sub>3</sub>; picrate, m. 224°; monoacetate, from Ac<sub>2</sub>O and H<sub>2</sub>SO<sub>4</sub> and crystallized from H<sub>2</sub>O, m. 174°; 2-benzylideneamino compound, prepared in hot BzH and crystallized from EtOH, m. 214° (decomposition). 5-Carbethoxy-2-methyl-G, prepared in 0.1-g. yield from 2.5 g. I and 2.9 g. MeC(:NH)OEt 24 h. in Et<sub>2</sub>O at room temperature, m. 167° (decomposition) (from EtOH-Et<sub>2</sub>O); the HCl salt (65% from I and MeC(:NH)SCH<sub>2</sub>Ph.HCl refluxed 4 h. in CHCl<sub>3</sub>), m. 213-14° (decomposition), was easily converted to the free base. Addition of 5.6 g. HC(:NH)NH<sub>2</sub>.HCl with just sufficient EtOH for solution to 9 g. I in 200 cc. CHCl<sub>3</sub>, 2 h.' refluxing, 12 h.' standing of the blackened solution at room temperature, filtration from the 80% yield of NH<sub>4</sub>Cl, addition of Et<sub>2</sub>O to turbidity, filtration of a black oil after 6 h. at 0°, and concentration in vacuo gave 40% 5-carbethoxy-G, m. 180-1° (from EtOAc-EtOH). This product could not be prepared from HC(:NH)OEt or HC(:NH)OCHMe<sub>2</sub>. 5-Phenyl-2-benzyl-G, obtained in 45% yield by 12 h.' refluxing of 3 g. II and 1.7 g. PhCH(NH<sub>2</sub>)CN (III) in CHCl<sub>3</sub>, filtration of 3 g. HCl salt (m. 200° with decomposition), and liberation of the free base in the min. of warm H<sub>2</sub>O with NaOH, m. 199° (from MeOH); picrate, m. 215°; di-Ac derivative, m. 215° (from MeOH). PhC(:NH)SCH<sub>2</sub>Ph (2 g.) and 1 g. III similarly gave 1 g. 2,5-diphenyl-G, a white solid rapidly turning green; picrate, m. 220° (from EtOH). MeC(:NH)SCH<sub>2</sub>Ph.HCl (5 g.) and 3.5 g. III in boiling CHCl<sub>3</sub> gave 5 g. crystalline product, very soluble in H<sub>2</sub>O and MeOH, insol. in Me<sub>2</sub>CO, and not diazotized in dilute HCl. It m. 125° on rapid heating, but 15 mins.' heating at 200° gave 5-phenyl-2-methyl-G.HCl, m. 238° (from MeOH), diazotizable in dilute HCl. Refluxing 1.2 g. 5-carbethoxy-2-benzyl-G 1 h. with 0.4 g. MeNCS in 5 cc. C<sub>5</sub>H<sub>5</sub>N, addition of H<sub>2</sub>O, and crystallization of the precipitate from EtOH gave 1.3 g. 5-carbethoxy-2-benzyl-MTG (MTG = 4-(3-methyl-2-thioureido)glyoxaline, m. 174°, converted by warming 1 min. in 10% NaOH and addition of excess HOAc to gelatinous 2-thio-8-benzyl-MX (MX = 1-methylxanthine). Similarly prepared, 5-carbethoxy-2-phenyl-MTG, m. 245°, converted by NaOH to 2-thio-8-phenyl-MX. 5-Carbethoxy-2-phenyl-G and MeNCO instead of MeNCS gave 5-carbethoxy-2-phenyl-MUG [MUG = 4-(3-methylureido)glyoxaline], m. 181-2°, converted by alkali to the corresponding 8-phenyl-MX; the latter was also formed by the action of H<sub>2</sub>O<sub>2</sub> on 2-thio-8-phenyl-MX in 5% NaOH at 0° one week and then boiling and addition of excess HOAc. 5-Carbethoxy-2-methyl-MTG, prepared as above, m. 194° (from EtOAc), gave the 2-thio-8-methyl-MX. 5-Carbethoxy-2-methyl-G and MeNCO in C<sub>5</sub>H<sub>5</sub>N were refluxed 2 h., concentrated in vacuo, and the residue converted with alkali, etc., to 8-methyl-MX. 5-Carbethoxy-MTG, m. 163°, was converted to the 2-thio-MX. Addition of 0.5 g. KClO<sub>3</sub> during 30 min. to 2 g. 8-phenyl-MX in 2.7 cc. concentrated HCl and 5 cc. H<sub>2</sub>O below 60° maintenance at 0° 1 h., filtration from the 0.6 g. precipitate, aeration for 3 h. to remove excess Cl, addition of 1.3 g. SnCl<sub>2</sub> in 1 cc. concentrated HCl during 30 min. at 0 to -5°, and standing 12 h. at 0° gave 0.4 g. dimethylalloxantin, m. and mixed m.p. 200° (to a red liquid). This was converted by boiling with aqueous o-C<sub>6</sub>H<sub>4</sub>(NH<sub>3</sub>Cl)<sub>2</sub> to 3-methylalloxazine, m. and mixed m.p. 280° (decomposition) (from HOAc-EtOH). 8-Methyl-MX similarly oxidized and reduced gave dimethylalloxantin, m. 207° (from H<sub>2</sub>O).

IT 91184-08-6P, Xanthine, 1-methyl-2-thio- 874519-01-4P,

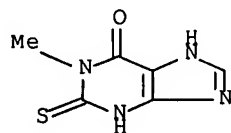
Xanthine, 1,8-dimethyl-2-thio-

RL: PREP (Preparation)

(preparation of)

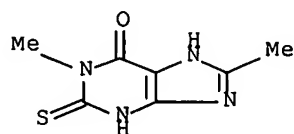
RN 91184-08-6 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1-methyl-2-thioxo- (9CI) (CA INDEX NAME)



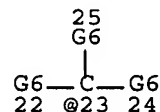
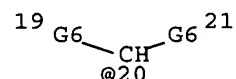
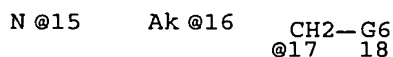
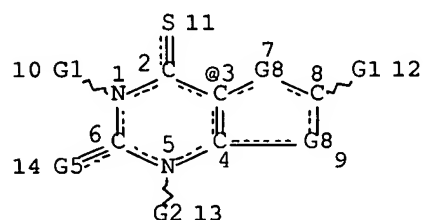
RN 874519-01-4 CAPLUS

CN Xanthine, 1,8-dimethyl-2-thio- (5CI) (CA INDEX NAME)

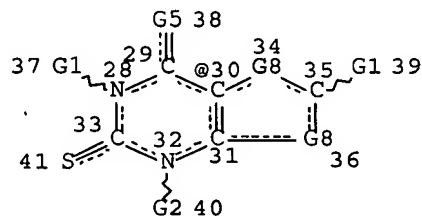


FILE 'HOME' ENTERED AT 15:03:12 ON 12 MAR 2007

=> d stat que l7; d his nofile  
L4 STR



O @27



G7 42

C @43

N—Ak  
@44 45

VAR G1=H/16  
VAR G2=H/ME/17/20/23  
VAR G5=O/S  
VAR G6=27/43  
VAR G7=3/30  
VAR G8=15/NH/44  
NODE ATTRIBUTES:  
NSPEC IS RC AT 27  
NSPEC IS RC AT 43  
CONNECT IS X3 RC AT 8  
CONNECT IS E2 RC AT 15  
CONNECT IS E1 RC AT 16  
CONNECT IS X3 RC AT 35  
CONNECT IS E1 RC AT 45  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RSPEC I  
NUMBER OF NODES IS 44

STEREO ATTRIBUTES: NONE  
L7 242 SEA FILE=REGISTRY SSS FUL L4.

100.0% PROCESSED 366449 ITERATIONS  
SEARCH TIME: 00.00.04

242 ANSWERS

(FILE 'HOME' ENTERED AT 10:44:06 ON 12 MAR 2007)

## SEARCH HISTORY

FILE 'REGISTRY' ENTERED AT 10:44:32 ON 12 MAR 2007

D SAVED

ACT BER645FULL/A

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L1          STR
L2          258797 SEA SSS FUL L1
          -----
L3          STR L1
L4          STR L3
L5          1 SEA SSS SAM L4
          D SCAN
L6          366449 SEA SSS FUL L4 EXTEND
L7          242 SEA SSS FUL L4
          SAVE TEMP L7 BER537FULL/A

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FILE 'CAPLUS' ENTERED AT 11:23:54 ON 12 MAR 2007

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L8          444 SEA ABB=ON L7
L9          ANALYZE L8 1- RN HIT :      204 TERMS
          D

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FILE 'REGISTRY' ENTERED AT 11:25:35 ON 12 MAR 2007

```

L10         1 SEA ABB=ON 2002-59-7
L11         1 SEA ABB=ON 2487-40-3
L12         1 SEA ABB=ON 5437-25-2
L13         239 SEA ABB=ON L7 NOT (L10 OR L11 OR L12)

```

FILE 'CAPLUS' ENTERED AT 11:25:52 ON 12 MAR 2007

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L14         122 SEA ABB=ON L13
L15         410 SEA ABB=ON L8 AND (PY<2003 OR AY<2003 OR PRY<2003)
L16         117 SEA ABB=ON L14 AND L15

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FILE 'REGISTRY' ENTERED AT 11:26:51 ON 12 MAR 2007

FILE 'CAPLUS' ENTERED AT 12:15:58 ON 12 MAR 2007

E US2004-511537/APPS

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L17         1 SEA ABB=ON US2004-511537/AP
          D SCAN
          SEL RN

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FILE 'REGISTRY' ENTERED AT 12:16:34 ON 12 MAR 2007

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L18         79 SEA ABB=ON (102353-42-4/BI OR 105-56-6/BI OR 111538-46-6/BI
          OR 139460-80-3/BI OR 139460-81-4/BI OR 139460-82-5/BI OR
          1516-33-2/BI OR 263552-78-9/BI OR 37412-64-9/BI OR 405-74-3/BI
          OR 436094-96-1/BI OR 56541-07-2/BI OR 591-82-2/BI OR 59814-51-6
          /BI OR 618913-11-4/BI OR 618913-12-5/BI OR 618913-13-6/BI OR
          618913-14-7/BI OR 618913-15-8/BI OR 618913-16-9/BI OR 618913-17
          -0/BI OR 618913-18-1/BI OR 618913-19-2/BI OR 618913-20-5/BI OR
          618913-21-6/BI OR 618913-22-7/BI OR 618913-23-8/BI OR 618913-24
          -9/BI OR 618913-25-0/BI OR 618913-26-1/BI OR 618913-27-2/BI OR
          618913-28-3/BI OR 618913-29-4/BI OR 618913-30-7/BI OR 618913-31
          -8/BI OR 618913-32-9/BI OR 618913-33-0/BI OR 618913-34-1/BI OR
          618913-35-2/BI OR 618913-36-3/BI OR 618913-37-4/BI OR 618913-38
          -5/BI OR 618913-39-6/BI OR 618913-40-9/BI OR 618913-41-0/BI OR
          618913-42-1/BI OR 618913-43-2/BI OR 618913-44-3/BI OR 618913-45
          -4/BI OR 618913-46-5/BI OR 618913-47-6/BI OR 618913-48-7/BI OR
          618913-49-8/BI OR 618913-50-1/BI OR 618913-51-2/BI OR 618913-53
          -4/BI OR 618913-55-6/BI OR 618913-56-7/BI OR 618913-57-8/BI OR
          618913-58-9/BI OR 618913-59-0/BI OR 618913-60-3/BI OR 618913-61

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-4/BI OR 618913-62-5/BI OR 618913-63-6/BI OR 618913-64-7/BI OR  
 618913-65-8/BI OR 618913-66-9/BI OR 618913-67-0/BI OR 618913-68  
 -1/BI OR 63908-28-1/BI OR 66892-25-9/BI OR 66892-28-2/BI OR  
 66892-33-9/BI OR 6815-00-5/BI OR 75914-95-3/BI OR 75914-97-5/BI  
 OR 81250-28-4/BI OR 9003-99-0/BI)

D SCAN

E MYELOPEROXIDASE/CN

L19 1 SEA ABB=ON MYELOPEROXIDASE/CN

FILE 'REGISTRY' ENTERED AT 12:30:15 ON 12 MAR 2007

D IDE

FILE 'CAPLUS' ENTERED AT 12:31:34 ON 12 MAR 2007

L20 1 SEA ABB=ON L17 AND L8

FILE 'CAPLUS' ENTERED AT 12:31:52 ON 12 MAR 2007

D IBIB ED ABS HITSTR

L21 42778 SEA ABB=ON L19

L22 1 SEA ABB=ON L21 AND L8

D SCAN

L23 4978 SEA ABB=ON NEUROINFLAM?/OBI OR (NERV?/OBI OR NEURON?/OBI) (L) IN  
 FLAM?/OBI

L24 1 SEA ABB=ON L23 AND L8

FILE 'REGISTRY' ENTERED AT 12:34:15 ON 12 MAR 2007

D QUE L7

L25 STR L4

L26 13 SEA SUB=L7 SSS SAM L25

D QUE NOS

L27 STR L4

D SCAN L10

D SCAN L11

D SCAN L12

L28 22 SEA ABB=ON L7 AND L18

L29 22 SEA ABB=ON L28 NOT (L10 OR L11 OR L12)

FILE 'CAPLUS' ENTERED AT 14:17:20 ON 12 MAR 2007

L30 2 SEA ABB=ON L29

FILE 'REGISTRY' ENTERED AT 14:17:55 ON 12 MAR 2007

D SCAN L29

FILE 'STNGUIDE' ENTERED AT 14:18:07 ON 12 MAR 2007

FILE 'REGISTRY' ENTERED AT 14:25:23 ON 12 MAR 2007

L31 21 SEA ABB=ON L7 AND CHOLINE

D SCAN

FILE 'CAPLUS' ENTERED AT 14:27:08 ON 12 MAR 2007

L32 3 SEA ABB=ON L31

FILE 'STNGUIDE' ENTERED AT 14:27:23 ON 12 MAR 2007

FILE 'CAPLUS' ENTERED AT 14:35:51 ON 12 MAR 2007

D SCAN L17

L33 48 SEA ABB=ON L8(L) (THU OR PAC OR BAC OR PKT OR DMA)/RL

L34 2186237 SEA ABB=ON PHARMAC?/SC, SX

L35 145 SEA ABB=ON L8 AND L34

L36 43 SEA ABB=ON L35 AND L14

L37 80 SEA ABB=ON L33 OR L36

FILE 'REGISTRY' ENTERED AT 14:39:47 ON 12 MAR 2007  
L38 1 SEA ABB=ON 2398-70-1  
L39 238 SEA ABB=ON L13 NOT L38

FILE 'CAPLUS' ENTERED AT 14:40:05 ON 12 MAR 2007  
L40 109 SEA ABB=ON L39

FILE 'STNGUIDE' ENTERED AT 14:41:29 ON 12 MAR 2007  
FILE 'REGISTRY' ENTERED AT 14:42:39 ON 12 MAR 2007  
D STAT QUE L8  
D IDE L10

FILE 'CAPLUS' ENTERED AT 14:44:19 ON 12 MAR 2007  
L41 192 SEA ABB=ON L10  
L42 122 SEA ABB=ON L41 NOT ((L11 OR L12 OR L13))  
L43 24 SEA ABB=ON L42 AND P/DT  
D IBIB ED ABS HITSTR 20-24

FILE 'REGISTRY' ENTERED AT 14:46:08 ON 12 MAR 2007  
D IDE L11

FILE 'CAPLUS' ENTERED AT 14:46:16 ON 12 MAR 2007  
L44 154 SEA ABB=ON L11  
L45 89 SEA ABB=ON L44 NOT ((L12 OR L10 OR L13))  
L46 52 SEA ABB=ON L45 AND P/DT  
D IBIB ED ABS HITSTR 48-52

FILE 'REGISTRY' ENTERED AT 14:47:20 ON 12 MAR 2007  
D IDE L12

FILE 'CAPLUS' ENTERED AT 14:47:27 ON 12 MAR 2007  
L47 48 SEA ABB=ON L12 NOT ((L10 OR L11 OR L13))  
L48 16 SEA ABB=ON L47 AND P/DT  
D IBIB ED ABS HITSTR 12-16

FILE 'REGISTRY' ENTERED AT 14:48:47 ON 12 MAR 2007  
D QUE NOS L7  
L49 STR L4  
L50 14 SEA SUB=L7 SSS SAM L49  
L51 STR L49  
L52 13 SEA SUB=L7 SSS SAM L51  
D SCAN  
L53 242 SEA SUB=L7 SSS FUL L51 EXTEND  
L54 212 SEA SUB=L7 SSS FUL L51  
SAVE TEMP L54 BER537SUB1/A  
L55 209 SEA ABB=ON L54 NOT (L10 OR L11 OR L12)

FILE 'CAPLUS' ENTERED AT 15:00:14 ON 12 MAR 2007  
L56 119 SEA ABB=ON L55  
D QUE NOS L16

FILE 'REGISTRY' ENTERED AT 15:02:06 ON 12 MAR 2007  
D STAT QUE L7

FILE 'CAPLUS' ENTERED AT 15:02:06 ON 12 MAR 2007  
D QUE NOS L16  
L57 116 SEA ABB=ON L16 NOT L17  
D IBIB ED ABS HITSTR 1-116

FILE 'HOME' ENTERED AT 15:03:12 ON 12 MAR 2007  
D STAT QUE L7

thione (IV), and 3-methyl-6-methylthiopurine (V) had C:N bonds fixed in the 1,2-position. This bond fixation alone was inadequate in explaining the rate of attack of these compds. by milk xanthine oxidase. 3-Methylxanthine (3 g.) was refluxed 2 hrs. with 15 g. P2S5 in 150 ml. C5H5N, the solvent evaporated, the residue heated with water (15 min.), and the pH brought to 9 with NH4OH. After 30 min., this solution was filtered, and the filtrate concentrated in vacuo to 50 ml. and acidified to pH 5.5 to precipitate 2.2 g. 2-hydroxy-3-methylpurine-6-thione (VI), which was purified by treatment with C in 5% NaOH, precipitated with HOAc, and recrystd. from water as yellow needles, decomposing above 300°. VI (1.2 g.) in 25 ml. N NaOH was refluxed 2 hrs. with 4 g. Raney Ni (VII), VII removed, and the solution evaporated to dryness. The residue was dissolved in 5% ethanolic H2SO4 and water added to just clarify the solution which, after treatment with C and storage at 0°, deposited 23% 3-methyl-2-purinone (VIII) as the sulfate in large colorless plates. VIII, colorless needles, decomposed 297-300° (EtOH). Similarly, 0.2 g. 3-methyl-6-thiouric acid refluxed 70 min. with 0.8 g. VII in 20 ml. 5% NH4OH gave, on acidification and cooling, 90 mg. 8-hydroxy-3-methyl-2-purinone, flat rods, decomposing above 300° (water). 1,2-Dihydro-1-methyl-2-thio-4-hydroxy-5,6-diaminopyrimidine (IX) (CA 55, 2656g) (3.3 g.) and 12 ml. HCONH2 heated 1.5 hrs. at 180-90° gave, on cooling, 3.2 g. 6-hydroxy-3-methylpurine-2-thione (X), prisms, decomposing above 300° (water). X (3 g.) was heated to 90° in 70 ml. 5% NH4OH, 9 g. VII added, and heating and stirring continued 2 hrs. to give, on cooling and concentration of the solution, 1.9 g. I, colorless needles, decomposing above 300° (50% EtOH) (crystallizing with 1/3 H2O). Heating 1 g. IX and 1 g. CO(NH2)2 20 min. at 195°, dissolving the product in 5% NaOH, treating with C, and acidifying with 20% H2SO4pptd. 90% 6,8-dihydroxy-3-methylpurine-2-thione (XI), decomposing above 300°. Desulfurization of XI in 10 ml. N NaOH (refluxed 1.5 hrs. with 1.5 g. VII) followed by acidification with 20% H2SO4 gave 0.3 g. II, colorless plates, decomposing above 300° (H2O). 2,6-Dimercapto-3-methyl-8-purinol (1 g.) in 10 ml. 2.5% NaOH was refluxed with stirring with 2 g. VII; after 45 min., 2 g. VII was added and refluxing continued 70 min. The filtrate was brought to pH 7.5 with HOAc, evaporated to dryness, and the residue extracted with cold EtOH. The residue was crystallized from hot 90% EtOH to give 250 mg. III, subliming about 250°, m. above 300°. Treatment of 0.8 g. XI with 2.5 g. P2S5 in 45 ml. C5H5N (as in the preparation of VI) gave 68% 2-mercapto-3-methylpurine-6-thione (XII), yellowish elongated prisms, decomposing above 300° (Me2NCHO-water). Refluxing 1.1 g. I with 5 g. P2S5 in 60 ml. C5H5N 4 hrs. gave, after evaporation of solvent and treatment with hot water, 0.8 g. IV, yellowish pointed prisms, decomposing above 300° (H2O). Treatment of 0.4 g. IV in 5 ml. 2.5% NaOH at room temperature with 0.3 ml. MeI (2 hrs.) gave 0.4 g. V, colorless prisms (water), m. 166°. IV, V, and XII could not be desulfurized to 3-methylpurine.

IT 28139-02-8P, Xanthine, 3-methyl-2-thio- 33285-76-6P,

Xanthine, 3-methyl-6-thio-

RL: PREP (Preparation)

(preparation of)

RN 28139-02-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)

